Computer simulation of the atomic structure of defects in metals

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The basic methods used in the computer simulation of the atomic structure and structural changes of defects in metals—molecular dynamics, variational procedures, and the lattice statics method—are briefly reviewed. There is a discussion of some new interatomic potentials, in particular, potentials which incorporate the partially filled d shells of transition metals. Some typical results of the calculations of the atomic structure of defects and their formation and migration energies are reported. These results refer to mixed dumbbells, complexes consisting of a vacancy and an impurity atom, clusters of vacancies and interstitial atoms, and dislocation cores in bcc and hcp metals, including transition metals, and in alloys with a long-range order; special grain boundaries; defects in void superlattices in irradiated metals; and point defects in amorphous metals. The future outlook for simulation is discussed.

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1. INTRODUCTION

It has been more than seven years since the computer simulation of defects in crystals was last reviewed in this Journal.¹ Many new results have been obtained since then, and computer simulation has become a more important method for research in solid state physics. Simulations were originally carried out primarily to study radiation-induced defects (as can be seen from the title of Ref. 1), but now the list of subjects being studied includes—along with the various point defects and their complexes—dislocations, grain boundaries, amorphous metals, and microcracks; and these entities are being studied not only in simple monatomic metals but also in transition metals, ordered and disordered alloys, and intermetallic compounds.

The speed and memory capacity of computers have improved substantially, making it possible to study comparatively large defects: not only their static structure but also the dynamics of their structural changes.

Progress in the theory of metals has made it possible to go beyond the binary central forces in the description of the interactions of atoms in a solid to take the electronic structure of the metal into account in a more systematic way. In particular, it has become possible to take into account the structural features due to the presence of conduction electrons and the unfilled d shells of transition metals. The "semidiscrete" model of a crystal with a defect, which takes explicit account of the atomic structure only in a small volume (the "core" of the defect), while the displacements of nearby atoms are calculated from the theory of elasticity, can be replaced by the model of lattice statics in which all the atoms of the crystal can be described discretely under appropriate periodicity conditions.

All this progress has substantially increased the list of entities and atomic structural changes which can be studied by computer simulation, and it has revealed the atomic mechanisms for many structure-sensitive properties of a variety of crystalline materials.

Although experimental methods for directly observing the structures of defects at the atomic level have been improved significantly in recent years (individual atoms have been directly resolved in the field-ion microscope; atomic planes and rows have been resolved in an electron microscope; the atomic configurations of point defects have been determined by diffuse x-ray scattering; Mössbauer spectroscopy has been developed; the methods of positron and muon annihilation have been developed; etc.), many details of the structures of defects remain beyond the resolution of these methods. Furthermore, experiments of this type require unique and expensive apparatus. Consequently, computer simulation has remained an indispensable tool for research in solid state physics. The increase in the volume of simulations is reflected in the fact that an All-Union Seminar on the Computer Simulation of Radiation-Induced and Other De-

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fects² has been meeting regularly since 1976, and international conferences have been convened. We are approaching a time when any actual experiment (especially an expensive one) in solid state physics will be preceded by a corresponding computer simulation.

Our purpose in the present review is to generalize the data on the defect structures of crystals which have been obtained since the review in Ref. 1. We will be able to discuss only certain typical studies in the space available here. The particular interests of the authors are of course reflected in the choice of topics. Some topics which are completely excluded are defects in nonmetallic crystals, the use of computers in quantum chemistry, the structure of crystal surfaces, growth processes, the structure and nucleation mechanisms of microcracks, and the kinetics of dislocations, in particular, their passage through a network of stops. Substantial progress has been made in each of these fields. We have attempted to avoid reproducing the material in monographs on defects in crystals and the material in the review of Ref. 1; we regard the present review as a continuation of Ref. 1. A popularized introduction to the subject is given in Ref. 4.

2. NUMERICAL METHODS FOR STUDYING THE ATOMIC STRUCTURE AND STRUCTURAL CHANGES OF DEFECTS

The first computer simulations of the atomic structures of defects were carried out by the Vineyard group^{5,6} for copper. Their model was based on a molecular dynamics method which had originally been proposed for studying the atomic structure of liquids⁷⁻⁹ but which subsequently proved to be the most flexible method for simulating defect structures and the formation, interaction, and migration of defects.

This model looks at a finite volume of the crystal (a "microcrystallite") around the initial, often hypothetical position of the atoms in the core of the defect (for example, in an analysis of the atomic structure of a vacancy, one of the atoms of the crystal is initially taken out of the crystal: its coordinates are assigned nearly infinite values). It is assumed that the atoms in this finite volume interact through binary central forces such as the Born-Mayer force, for example. The coupling provided by the conduction electrons in the metal is simulated by forces constantly directed inward at the atoms at the boundary of the volume under consideration. The rest of the crystal is assumed infinite and is replaced by an elastic continuum with elastic constants corresponding to the particular metal. The motion of the atoms in the microcrystallite is described by the classical equations. Additional boundary forces, elastic and viscous, are introduced at the boundary of the microcrystallite to simulate the response of the infinite elastic matrix. The size and shape of the microcrystallite are determined by the size and shape of the particular defect of interest. As we have already mentioned, the calculation of the atomic structure of a defect begins with the specification of the presumed configuration of the core of the defect, and it ends when the perturbation caused by the difference between this presumed configuration and the actual configuration has died out, and the defect has adopted an atomic structure which corresponds to a minimum of the potential energy. The large number of

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atoms in the microcrystallite (as many as several thousands in the calculations presently being carried out) and thus the large number of coupled equations of motion put this problem beyond the reach of analytic methods. Computers and thus numerical methods make the problem solvable.

The system of coupled equations of motion of the atoms of the microcrystallite is

$$\mathbf{\dot{r}}_{i}(t) = \mathbf{v}_{i}(t), \quad i = 1, 2, 3, \dots, N,$$

$$\mathbf{\dot{v}}_{i}(t) = m^{-i}\mathbf{F}_{i}[\mathbf{r}_{1}(t), \dots, \mathbf{r}_{N}(t); \mathbf{v}_{i}(t)], \qquad (1)$$

where $\mathbf{r}_i(t)$ is the coordinate of the *i*th atom at the time, t, $\mathbf{v}_i(t)$ is the corresponding velocity, N is the number of atoms in the microcrystallite, \mathbf{F}_i is a force which depends on the positions of all the atoms (and if the atom is a boundary atom, this force also depends on the velocity of the atom), and m is the mass of the atom. System (1) is usually integrated by one of the numerical methods available (the ordinary Euler method, the refined Euler method, the Euler-Cauchy method, the Runge-Kutta method, etc.). The choice of a particular method is governed by the size of the microcrystallite, the calculation accuracy required, and the capacity of the computer. A more detailed description of the modeling algorithms which have been developed on the basis of these principles can be found in Refs. 10–15.

The subsequent development of defect models based on molecular dynamics has taken the path of refinements in the interatomic potentials (we will take up this important topic in more detail below), incorporation of the thermal vibrations of the atoms of the microcrystallite, ^{13,16} and the introduction of more complicated boundary conditions, especially for large defects^{13,17} (dislocations, grain boundaries, and so forth).¹⁾

The thermal vibrations of the atoms of the microcrystallite had to be introduced in order to test the dynamic stability of the equilibrium atomic structures found for the defects in the quasidynamic regime at temperatures near absolute zero (the Vineyard model has all the atoms of the microcrystallite, except for those of the defect core, initially at rest at sites in an ideal crystal lattice).²⁾ The stability of the atomic structures of the defects in the algorithms presently used for the simulations is tested by assigning a random velocity vector (or an excursion from the equilibrium position) to each atom in the microcrystallite. The magnitude and direction of these vectors and a characteristic such as the correlation function are determined from the given temperature of the crystal containing the defect of interest.

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¹⁾Curiously, the methods which have been developed to simulate atomic structures of defects in crystals have proved useful for calculating the equilibrium configuration of macroscopic systems having a discrete periodic structure. In particular, these methods have been applied to "super-lattices" of vacancy pores and gas-filled pores which are observed in irradiated metals. In such superlattices there are "vacancies" (this means the absence of a pore from some "site") and "dislocations." By calculating the interaction potential of two pores as a function of the distance between them by elastic theory one can find the equilibrium configurations of the "defects" of the superlattice and compare them with the observed configurations.¹⁸

²⁾It would be more accurate to characterize this situation as the hypothetical case of a zero temperature, rather than the actual case, since the situation also lacks zero-point vibrations.

Refinements in the "joining" of the boundaries of the microcrystallite with the rest of the infinite crystal, replaced by an elastic continuum, get into the field of models which simulate the structures of defects with dimensions greater than those of the microcrystallite (the calculation cell).

In this situation the microcrystallite is broken up into two subsystems: a central calculation cell of mobile atoms (region 1), surrounded on all sides by a casing of immobile atoms (region 2). A preliminary structure for the defect is introduced in the form of a displacement field for this defect in the crystal lattice. This field is calculated by elastic theory. Before the simulating calculation, this approximate displacement field is specified in both regions 1 and 2 of the microcrystallite. When the calculation to simulate the extended defect is begun, the atoms of region 2 remain fixed, since elastic theory gives a rather accurate description of the atomic displacements far from the defect core, while the atoms in region 1 freely relax from their original approximate positions. Moving in accordance with the particular interatomic potentials and the laws of Newtonian mechanics, these atoms occupy positions which lead to the state with the lowest potential energy.

An even more complicated microcrystallite with periodic boundary conditions is used in several problems, especially for determining the atomic structure of line defects.¹³ The periodic boundary conditions are imposed at two (or four) opposite faces of the microcrystallite. Large defects such as edge dislocations or grain boundaries are arranged in the calculation cell along the normal to the faces with the periodic boundary conditions.

The extremely popular variational model^{17,19} differs from the dynamic model primarily in the method used for the numerical calculation of the stable atomic defect structures. Precisely as in the dynamic model, the atoms of a finite part of the lattice (a microcrystallite) are treated as particles which interact with each other. In the variational model the microcrystallite is usually a sphere. A central binary interatomic interaction φ^{ij} is given. The neighbors in the nearest coordination spheres are taken into account. The microcrystallite is surrounded by an elastic medium which contains the lattice atoms. Displacements of the elastic medium and of the atoms in it are described by the spherically symmetric vector field³⁾

$$\mathbf{u} = C \frac{\mathbf{r}}{r^3},\tag{2}$$

where C is a measure of the strength of the defect. In this model the volume increase due to the presence of the defect depends linearly on C. The energy of the microcrystallite is written as the sum

$$E = \frac{1}{2} \sum_{i} \sum_{j} \varphi^{ij} + \sum_{i} \sum_{k} \varphi^{ik} + aC + bC^{2}, \qquad (3)$$

where φ^{ij} is the potential of the interaction between atoms *i* and *j*, the summation over *j* is over all the atoms of the crystallite which interact with the *i*th atom, and the summation over *k* is over all the atoms of the exterior of the crystallite.

The term aC describes the work performed in opposing the forces required to hold the ideal lattice at equilibrium, while bC^2 is the energy of the elastic field.

The energy for some particular structure is found from the difference $E - E_0$, where E_0 is the energy of the ideal lattice containing the same number of atoms:

$$E_0 = \frac{1}{2} \sum_i \sum_j \varphi_0^{ij} + \sum_i \sum_k \varphi_0^{ik}, \qquad (4)$$

where the subscript 0 means that the given term is calculated for the defect-free lattice.

The force exerted on the *i*th atom by the *j*th atom is

$$\mathbf{F}^{ij} = \frac{\mathrm{d}\boldsymbol{\varphi}^{ij}}{\mathrm{d}\boldsymbol{r}^{ij}} \frac{\mathbf{r}^{ij}}{\boldsymbol{r}^{ij}},\tag{5}$$

where $\mathbf{r}^{ij} = \mathbf{r}^i - \mathbf{r}^j$. The total force exerted on the *i*th atom is

$$\mathbf{F}^{i} = \frac{\mathrm{d}E}{\mathrm{d}\mathbf{r}^{i}} = \sum_{i} \mathbf{F}^{ij} + \sum_{k} \mathbf{F}^{ik}.$$
 (6)

The generalized force which is exerted on the crystallite and which is associated with the elastic variable C is found from

$$F^{C} = -\frac{\mathrm{d}E}{\mathrm{d}C} = \sum_{i} \sum_{k} \mathbf{F}^{ik} \frac{\mathrm{d}r^{k}}{\mathrm{d}C} - a - 2bC.$$
(7)

The energy minima and saddle points are determined in the following way: Some initial configuration is selected, and the initial vector positions of each atom in the microcrystallite are specified. Each coordinate of each atom is then changed in turn until the component of the corresponding force exerted on the *i*th atom vanishes. The elastic variable *C* is then given the value which makes the generalized force vanish, $F^{C} = 0$. The energy of the crystallite is calculated after each such cycle. Ordinarily, from 1 to 20 such iteration cycles are carried out.

A significant point here is that the dynamic relaxation procedure used in the dynamic model allowed the atoms to assume the minimum-energy configuration essentially at once. The static relaxation procedure used in the variational model reveals just which configuration has the minimum energy only after the energies of the various possible meta stable configurations have been calculated.

The partitioning of the crystal into a microcrystallite in which the positions of all the atoms are found by minimizing the energy and a peripheral zone, where the atomic positions are determined by elastic theory, suffers from the shortcoming that the boundary conditions influence the defect structure, and the influence increases as the microcrystallite becomes smaller. In the case of large defects (large on the atomic scale), it is not possible to eliminate completely the effect of the boundary conditions because of the limited memory and speed of computers.

A method which is free of this shortcoming is the lattice statics method, also called the method of static-displacement waves, proposed by Kanzaki²⁰ and Krivoglaz.²¹ Let us examine this approach. In general, when a crystal contains defects such as vacancies, interstitial atoms, or impurity atoms with a concentration c, the average positions of the atoms form a regular crystal lattice in which the site of index γ in cell s has a radius vector \mathbf{R}_{sy} . Concentration fluctuations δc cause the atoms to undergo disordered displacements \mathbf{u}_{sy} ,

³⁾Why this particular solution of the equilibrium equation in an isotropic elastic medium is adopted for describing u is discussed in detail in Ref. 27.

so that the actual coordinates of an atom, $s\gamma$, are $\mathbf{R}_{s\gamma} + \mathbf{u}_{s\gamma}$. We expand $\mathbf{u}_{s\gamma}$ in a Fourier series; i.e., we write it as a superposition of the amplitudes $\mathbf{u}_{k\gamma}$ of static-displacement waves (N is the number of sites in the crystal):

$$\mathbf{u}_{s\gamma} = i \sum_{h} \mathbf{u}_{h\gamma} e^{-ihR_{s\gamma}}, \quad \mathbf{u}_{h\gamma} = -\frac{i}{N} \sum_{s=1}^{N} \mathbf{u}_{s\gamma} e^{ihR_{s\gamma}}. \tag{8}$$

The distribution of defects among lattice sites $R_{s\gamma}$ is characterized by numbers $c_{s\gamma}$ which are equal to 1 if there is a defect at site $s\gamma$ or 0 if the site is occupied by a regular atom. By analogy with (8) we can replace the $c_{s\gamma}$ by their Fourier components,

$$c_{sy} - c = \sum_{k} c_{ky} e^{-ikR_{sy}}, \qquad (9)$$

where the $c_{k\gamma}$ are the amplitudes of the defect "concentration waves." Since the sources of the displacements are defects, we set (for simplicity we will omit the index γ below)

$$\mathbf{u}_k = \mathbf{A}_k c_k. \tag{10}$$

The amplitudes \mathbf{u}_k are determined from the condition for equilibrium of the lattice. In the macroscopic approximation, these amplitudes are

$$\sigma_{ij}n_j = 0, \tag{11}$$

where $\mathbf{n} = \mathbf{k}/k$,

$$\sigma_{ij} = \frac{\partial F^0}{\partial u_{ij}} = \lambda_{ijlm} \left(u_{lm} - L_{lm} \delta c \right) \tag{12}$$

are the components of the stress tensor, the u_{lm} are the strain components, F^0 is the free energy of the crystal, the λ_{ijlm} are components of the elastic-modulus tensor of the medium with an average defect concentration c, and the terms $L_{lm}\delta_c$ reflect the stresses caused by the defect concentration fluctuations δ_c . In the long-wave limit (small values of k) we then find²²

$$\mathbf{A}_{k} = \frac{a_{k} \mathbf{e}_{k}}{k} \,, \tag{13}$$

where \mathbf{e}_k is some unit vector, and a_k depends on the direction but not the magnitude of **k**. In the simplest case of an isotropic continuum we would have

$$\mathbf{A}_{k} = a_{0} \frac{\mathbf{k}}{k^{2}}, \qquad a_{0} = \frac{1+\nu}{3(1-\nu)} \frac{1}{\nu} \frac{\partial \nu}{\partial c}, \quad \mathbf{e}_{k} = \mathbf{n},$$
(14)

where $a_k = a_0$ is independent of k, determined only by the c dependence of the volume (or the lattice constant). Also, v is the Poisson ratio.

For short fluctuation wavelengths, Eq. (10) remains in force, but in order to determine A_k we need to replace (11) by the equilibrium condition of the microscopic theory of lattices (the approach is similar to that taken in the theory of the thermal vibrations of crystals). For this purpose we write the free energy as

$$F = F_0 - \sum_{s, s'=1}^{N} w_{ss'i} (c_s - c) u_{si} + \frac{1}{2} \sum_{s, s'=1} v_{ss'ij} u_{si} u_{s'j}, \quad (15)$$

where w_{ss} , determines the force exerted by a defect at site s' on an atom at site s (the "Kanzaki force"), while $v_{ss'ij}$ determines the interaction between atoms s and s'. From the equilibrium condition

$$f_{si} = 0 = -\frac{\partial F}{\partial u_{si}} \tag{16}$$

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we find the system of equations

$$Q_{hij}A_{hj} = P_{hi}$$
 (i = 1, 2, 3)

for determining the coefficients A_k . In (17),

$$Q_{hij} = \sum_{s'=1}^{N} v_{ss'ij} \exp\left[i\mathbf{k}\left(\mathbf{R}_{s} - \mathbf{R}_{s'}\right)\right], \qquad (18)$$

(17)

$$P_{ki} = -i \sum_{s'=1}^{N} w_{ss'i} \exp\left[i\mathbf{k} \left(\mathbf{R}_{s} - \mathbf{R}_{s'}\right)\right].$$
(19)

If we restrict the discussion to the interactions $v_{ss'}$ and $w_{ss'}$ in only the nearest coordinate spheres, we can keep the number of terms in (18) and (19) small, and we can determine Q_{kij} and P_{ki} without difficulty. Solving system (17), and using (13), we can find the displacements of all the atoms from (8) without resorting to the concept of a hypothetical microcrystallite. As the c_k in (10) we should use the values corresponding to the given distribution of point defects. For example, for an isolated defect at the site $\mathbf{R}_s = 0$ we would have $c_s = 1$ and $c_{s'} = 0$ ($s \neq s'$), so that we would have $c_k = 1/N$.

Krivoglaz²² gives examples of calculations of this type which have been carried out for simple point defects even without the use of computers. Some new results are reported in Ref. 23. This method has been generalized to extended defects (dislocation cores).²⁴

We see that any of these methods for simulating defects requires some interatomic potential φ_{ii} [in (15), the derivatives of φ_{ii} appear in the expressions for w and v]. The dependence of φ_{ii} on the distance (r_{ii}) between atoms i and j is assumed known. Whether the energy E can be written as the sum of the energies of binary interactions (3), and whether the dependence $\varphi_{ij}(r_{ij})$ can be determined, is the subject of an extensive literature,²⁵⁻²⁹ but only binary central potentials have been used until recently. There are theoretical methods available for determining them; these methods work from an approximate solution of the quantum-mechanical problem of calculating the energy of the crystal. There are also empirical methods, in which $\varphi_{ii}(r_{ii})$ is taken to be a polynomial, a spline,³⁰ or some other function [for example, the Morse function $\varphi(r) = D(e^{-2\alpha(r-r_0)} - 2\alpha e^{-\alpha(r-r_0)})$, where D, α , and r_0 are constants], and the constants in the potentials are chosen in such a manner that the values calculated from the function $\varphi(r)$ for the energy of the defect-free crystal, the elastic constants, the lattice constant, and other characteristics agree with the experimental values. So far, the empirical potentials have been more reliable than the theoretical potentials.

We turn now to some recent results which have not been covered in the reviews we cited earlier.

The potentials which have been used in most studies are generally cut off between the second and third coordination spheres, although the interactions of conduction electrons are manifested over far greater distances. These interactions are incorporated in the pseudopotential theory, but this theory has not yet been developed very far for transition metals or noble metals. Consequently, attempts have been made to determine the shape of a binary potential not limited by a cutoff condition, by working from experimental data on the phonon spectra: the dependence of the frequencies of longitudinal (ω_1) and transverse (ω_{c1}, ω_{c2}) vibrations of the atoms

on the phonon wave vector k. The method for determining the relationship between the frequencies $\omega(\mathbf{k})$ and the derivatives of the energy of the binary interaction is discussed in Ref. 31, for example; the values of the coefficients c_{ii} in the expression for the potential between the (i - 1)st and *i*th coordination spheres, $E_i(r) = \sum_{i=1}^{s} c_{ii}(r - r_i)^{j-1}$, are given in Ref. 32 (they were determined from the phonon spectra of 18 cubic metals). The E(r) curves constructed from these coefficients are noticeably different from those found by other workers, e.g., in Refs. 17, 33, and 34, and some of this other work has made use of data on the phonon spectra. The reasons for the discrepancies lie in both the arbitrary assumptions (the cutoff of the potential at a short distance) and the use as adjustable parameters of [in addition to the curves $\omega(\mathbf{k})$ the vacancy formation energy (this approach gives rise to a very deep potential minimum between the radii of the first and second coordination spheres). Vacancies and other defects with high gradients of the electron density (the core of an edge dislocation, a microcrack, or the surface of the crystal) are described poorly by the potentials which are constructed from the properties of a defect-free crystal and which are suitable for a uniform distribution of the average electron density. In contrast, such potentials are useful for describing the core of a screw dislocation, stacking faults, grain boundaries, and amorphous metals.

To write the crystal energy E as the sum of the energies E_{ij} of the binary central interactions between atoms i and j is a rather crude approximation. Attempts have been made to refine it in several ways: 1) by incorporating in the energy of the metal terms which represent conduction electrons and which depend on the volume of the crystal; 2) by using terms which depend on the relative displacements of atoms along the normal to the line connecting them in the equilibrium configuration (in other words, terms which depend on the valence angles θ). These terms are important not only in covalent crystals but also in transition metals with unfilled d shells.

In the simple free-electron model, the energy of the conduction electrons, E_e , can be written as a sum of terms (representing the Coulomb, kinetic, exchange, and other energies) each of which has its own dependence on the volume of the metal, $V = V_0 + \Delta V$ (V_0 is the equilibrium value of V). If we retain the first few nonvanishing terms in the expansion $E_e(V)$ then the equilibrium condition $\partial E / \partial V = 0$ leaves us with $E_e(V) = E(V_0) + \alpha \Delta V^2$. Baskes and Melius³⁵ suggested using E_e in this form in the expression for the total energy of the crystal:

$$E = E_{\Sigma} + C' + \alpha \, \Delta V^2, \tag{20}$$

Where E_{Σ} is the sum of the energies E_{ij} of the binary interactions, described by splines $\Sigma_i a_i r^i$, and C' and α are additional constants in the potential. Working from experimental data on the lattice constants, binding energies, elastic constants, vacancy formation energies, vacancy migration energies, and other properties (ten in all) of Ni, Ag, Au, Pt, Pd, Cu, and Al, Baskes and Melius determined ten constants of the potential, including C' and α . They found satisfactory agreement with the experimental value of the formation energy of an interstitial atom and a Frenkel' pair, the formation energy of a divacancy, the migration energy of a divacancy, etc.

In order to take noncentral forces into account it becomes necessary to incorporate in the total energy of the crystal terms proportional to $\Delta \theta^2$, where θ is the deviation of the valence angle from its equilibrium value. This approach is taken in, for example, the theory of Ref. 6 for the lattice heat capacity. The need to take noncentral forces into account in computer simulation of defects in metals was realized only recently in a calculation of the energies of vacancies and dislocation cores in transition metals in which the covalent components are significant in the balance of forces of the binding. The approaches taken to calculate the binding energies of transition metals proved useful.^{37,38} This binding energy is determined primarily by the d electrons and can be written in the following form with the help of the moment method of Refs. 39 and 40:

$$\bar{e}_{0} = \int_{0}^{\varepsilon_{\mathrm{F}}} \varepsilon n_{i}^{0}(\varepsilon) \,\mathrm{d}\varepsilon = -10 \,\sqrt{\frac{z}{2\pi}} \mid \beta \mid e^{-\varepsilon_{\mathrm{F}}^{02}/2z\beta^{2}}, \qquad (21)$$

where z is the coordination number, ε_F^0 is the Fermi energy, and n_i^0 is the state density in the d band, which can be approximated by the Gaussian curve

$$n_i^0(\varepsilon) = (2\pi\mu_{2i})^{-1/2} \exp\left(-\frac{\varepsilon^2}{r\mu_{2i}}\right),$$

The second moment of the function can be written in the form³⁹

$$\mu_{2i} = \sum_{j=1}^{z} \beta_{ij}^{z}, \qquad (22)$$

where the effective resonance integral β_{ij} is expressed in terms of the Slater two-center integrals dd σ , dd π , and dd δ :

$$\beta_{ij}^2 = \frac{1}{5} \left[dd\sigma^2(ij) + 2 dd\pi^2(ij) + 2 dd\delta^2(ij) \right].$$
(23)

In a defect-free crystal with an interatomic distance R, all the β_{ij}^2 are equal to $\beta^2(R)$; expression (21) follows. Writing $\beta(R)$ in the form $\beta_0 e^{-qR}$, and adding to (21) the repulsion energy of the ion cores, which can be written in the form $\overline{\epsilon}_R = (1/2)zC_0e^{-pR}$ (C_0 and p are constants), we find the following expression for the binding energy per atom:

$$E_{\mathbf{c}} = 10 \, \sqrt{\frac{z}{2\pi}} \mid \beta \mid e^{-\varepsilon \frac{\theta^2}{\mathbf{F}}/2z\beta^2} \left(1 - \frac{q}{p}\right). \tag{24}$$

If the symmetric arrangement of atoms near a defect is disrupted, and the atoms are displaced by u_i and u_j , all the integrals in (23) change. We write β_{ij} as $\beta_{ij} = \beta (1 + \theta_{ij})$, where

$$\theta_{ij} = 2q \left[-d_{ij} - \frac{1}{2R} \left(u_{ij}^2 - d_{ij}^2 \right) + q d_{ij}^2 \right],$$
(25)

 $u_{ij} = |\mathbf{u}_i - \mathbf{u}_j|, d_{ij} = (\mathbf{u}_i - \mathbf{u}_j) \times \mathbf{R}_{ij}/R$ and \mathbf{R}_{ij} , is the distance between atoms *i* and *j* in the defect-free crystal. Calculations which we will not reproduce here lead to an expression for $\delta \varepsilon_i(\mathbf{u}_i, \mathbf{u}_j)$, the change in the energy of the *i*th atom; this change depends on only the relative displacements of the nearest-neighbor atoms. This expression has been used to calculate the equilibrium configuration and energy of a vacancy⁴⁰ and of a dislocation core⁴² in a transition metal.

Although the modern electronic theory of metals gives a qualitatively correct description of most aspects of the interatomic interactions, even in comparatively complex systems, this theory is not yet capable of providing a quantitative description of these interactions which is accurate and reliable enough for use in computer simulation of defects. For the time being, it is thus necessary to work with empirical potentials (not necessarily central binary potentials) which incorporate as many as possible of the effects of interest; examples are the methods of Refs. 35 and 39.

The formation energy of certain point defects in noble metals was recently calculated by a potential incorporating three-particle interactions.¹⁵⁸

3. ATOMIC STRUCTURE AND INTERACTIONS OF POINT DEFECTS AND SMALL DEFECT CLUSTERS

a) Structures of point defects.

The simplest point defects are vacancies (an unoccupied site in a crystal lattice), interstitial atoms (a matrix atom in an interstitial position), substitutional impurities, and interstitial impurities.

New information on the atomic structure of these defects has been found by computer simulation. In several cases, this new information has forced a reexamination of existing ideas. For example, the specific displacement field of the atoms near vacancies in cubic metals has been found. As predicted by the elastic theory, the first neighbors are displaced toward the vacant site a distance which amounts to a few percent of the lattice constant. In copper, for example, this displacement is 1.5-3.2% (the spread results from the different interatomic potentials). The second nearest neighbors are not displaced toward the vacancy, as expected, but away from it, although the magnitude of the displacement is less than that for the first nearest neighbors.⁵ This anomalous relaxation is determined completely by the geometry of the crystal lattice. In contrast with an isotropic elastic continuum, the nearest neighbors in an fcc lattice, in being displaced toward the vacancy pushed the second nearest neighbors away from it. A similar displacement pattern has been found in a bcc metal (α iron).^{43,11} In an hcp metal (magnesium) it has also been found that the directions and magnitudes of the atomic displacements depend on the lattice geometry⁴⁴ (Fig. 1).

For an interstitial atom the most favorable configuration from the energy standpoint is a dumbbell oriented along the (100) direction in an fcc metal⁵ and along the (110)



FIG. 1. A vacancy (the dashed circle) and a trigonal interstitial atom (filled circle) in an hcp metal (magnesium).⁴⁴ Here $n^{(v)}$ is the *n*-th nearest enighbor of the vacancy, and $n^{(t)}$ is the *n*th nearest neighbor of the interstitial atoms.

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FIG. 2. Six configurations of a interstitial atom in α -iron.¹⁷ a– I_1 , (100) dumbbell; b– I_2 , (101) dumbbell; c– I_3 , crowdion; d– I_4 , displaced crowdion; e– I_5 , octahedral interstitial atom; f– I_6 , tetrahedral interstitial atom.¹⁷

direction in a bcc metal^{43,17} (Fig. 2b and Table I). A trigonal interstitial position is the most stable in hcp metals, although the less stable octahedral configuration has also been observed (Fig. 1).

The dumbbell configuration of interstitial atoms has now been confirmed by many experiments, and its reality is no longer in question.⁴⁵ The transition of a crowdion into a dumbbell, on the other hand, is still being debated.^{46,47}

b) Recombination of Frenkel' pairs.

The molecular dynamics method has made it possible to follow the changes in atomic structure in reactions between point defects. The most interesting reaction here has been the recombination of a Frenkel' pair. Knowing the atomic structures of a vacancy and an interstitial atom, and placing these two entities at various separations, we can determine that critical separation at which they begin to spontaneously move toward each other and recombine. The first study⁵ of the spontaneous-recombination zone in an fcc copper crystal revealed that the recombination zone around an interstitial dumbbell in the {100} plane is oriented along the (110) direction and contains 16 unstable sites; when a vacancy reaches one of these sites it spontaneously recombines with an interstitial atom. The recombination zone in copper was determined more comprehensively in three dimensions by Scholz and Lehmann⁴⁸ and Drittler et al.⁴⁹ Working with different potentials, these two groups found approximately equal numbers of unstable sites (74 and 62, respectively).

The zone in which Frenkel' pairs recombine in bcc crystals has been studied by several groups.^{43,50,51} It was mentioned in these papers that the recombination zone is very

TABLE I. Interstitial configurations in α -iron (Ω is the atomic volume).¹⁷

Con- figuration (Fig. 2)	Difference between the formation energies of the given configurationand of the , configuration, eV	Increase in thevolume of the crystal,
$ \begin{array}{c} I_1\\ I_2\\ I_3\\ I_4\\ I_5\\ I_6\\ I_7 \end{array} $	$\begin{array}{c} 1,29\\ 0\\ 0,32\\ 0,36\\ 1,12\\ 0,85\\ 0,33 \end{array}$	$1.7 \\ 1.6 \\ 1.7 \\ 1.7 \\ 1.4 \\ 1.5 \\ 1.7 $

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FIG. 3. Zone in which a Frenkel' pair recombines in the hcp lattice of magnesium.⁵² The filled circles are unstable positions of the vacancy. Shown here are five different (0001) planes, at various distances from the trigonal interstitial atom: a—0.2; b—1.4; c—0.6; d— 0.2; e—1.0. the interstitial atom lies between planes c) and d); its projection onto the plane d) is shown by the open circle.

anisotropic and has relatively small dimensions (a few tens of atoms). It has been found that the annihilation occurs in two ways. At the distance of the first neighbors, an interstitial atom immediately fills a vacancy. At greater distances the vacancy is filled by a nearest neighbor, not by the original interstitial atoms, whose motion towards the vacancy stimulates a small chain of atomic substitutions.

The lattice symmetry was found to have a significant effect on the recombination zone in an hcp metal (magnesium),⁵² where close-packed directions were identified ([11 $\overline{2}$ 0], [11 $\overline{2}$ 3]); these directions create channels for recombination. Analysis of the reaction of an interstitial atom in the most stable trigonal configuration with a vacancy revealed that a vacancy would recombine with any of 49 sites if it reached them (Fig. 3).

The size and shape of the zone in which Frenkel' pairs spontaneously recombine are affected by an external stress. In particular, hydrostatic compression increases the size of the zone.⁵¹ Uniaxial compression along any of various crystallographic directions also causes the recombination zone to grow,⁵³ but the growth occurs primarily perpendicular to the compression direction.

c) Defect clusters.

Computer simulations can be used to study systematically the atomic structure of clusters of vacancies and interstitial atoms as a function of the number (n) of defects in the cluster. It turns out that *n* cannot be regarded as an exhaustive characteristic of the cluster: Clusters with identical values of *n* may have different atomic structures. In an fcc lattice, for example, a cluster of two interstitial atoms⁵⁴ has a minimum of three stable⁴⁾ atomic configurations (Fig. 4). The energy of the interstitial clusters per atom, E_{ni}^{f}/n , is lower for compact equiaxial clusters in copper at small values of *n*, while at n > 9 it is lower for planar clusters.⁵⁵ Va-



FIG. 4. Various atomic configurations of a pair of interstitial atoms in an fcc copper crystal; these configurations have different binding energies⁵⁴: $\mathbf{a} - E_{2i}^{B} = 0.36 \text{ eV}; \mathbf{b} - E_{2i}^{B} = 40 \text{ eV}; \mathbf{c} - E_{2i}^{B} = 49 \text{ eV}.$

$$E_{ni}^{\mathbf{B}} = nE_{i}^{\mathbf{f}} - E_{ni}^{\mathbf{f}},$$

where *n* is the number of elementary defects of type *i* in the cluster, E_i^t is the formation energy of a single defect of type *i*, and E_{ni}^t is the formation energy of clusters of *n* atoms.

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cancy clusters are no exception to this rule (Fig. 5). A divacancy in a cubic crystal, for example, has several stable configurations. Calculations of the configurations of divacancies in α -Fe by a dynamic method with the potential of Erginsoy *et al.*⁴³ yield the following binding energies for two vacancies which are separated by the distances corresponding to the first, second, and third neighbors: 0.209, 0.47, and 0.097 eV, respectively.⁵⁶

With increasing number of defects in a cluster, the number of different atomic configurations of the cluster also increases. The definition of a cluster as a group of interacting defects does little to slow this proliferation, since a pair of vacancies, for example, will interact even at a distance greater than that corresponding to the tenth neighbor, and any large vacancy cluster could be arbitrarily broken up into such pairs. The number of possible configurations is usually restricted by considering only the most stable clusters (those with the largest binding energies).

To identify these most stable clusters one determines the binding energy of a pair of defects as a function of the distance between them. Calculations of this type carried out⁵⁷ for a divacancy in α -Fe (with the Johnson interatomic potential¹⁷) have shown that the binding energies at distances greater than that corresponding to the tenth neighbor $(d > d_{10})$ are less than 0.01 eV. It is thus a good approximation to restrict the interaction region for a pair of vacancies to tenth neighbors under the condition that the crystal temperature satisfies $T \ge 120 K$ ($kT \ge 0.01 eV$). At higher temperatures, the interaction region of two vacancies is even smaller. If we assume that vacancies migrate through α -Fe only above 250 °C (523 K), then in analyzing the diffusion of divacancies and their combination into clusters we may assume that the interaction region is approximately limited by the sixth neighbors (Table II).57

Even when restrictions of this sort are introduced, the number of different clusters still remains quite large. "Computer experiments" are absolutely necessary for analyzing and classifying the atomic configurations of these clusters. Although such calculations are being carried out extensively at present, only the most general tendencies in the evolution of the atomic configurations of clusters as a function of the number of defects, n, have been identified.

Vacancy clusters containing up to 38 vacancies have been studied in bcc crystals (for the particular case of α -Fe).⁵⁷ Calculations have been carried out for linear, planar, and compact (three-dimensional) clusters consisting of identical numbers of vacancies. It has been established that the cluster with the largest binding energy per vacancy is always the compact form. Figure 6 shows the stages in the growth and the various configurations of such clusters.

The binding energy of [110] two-layer plates of vacan-

⁴⁾A "stable configuration" of a cluster is its atomic configuration which has a positive binding energy



FIG. 5. Configurations of vacancy clusters in an fcc lattice.⁵⁴ The asterisks represent atoms which have undergone a large displacement during the formation of a stable configuration. The binding energies of the tetravacancies are a—0.1 eV (this is an unstable configuration); b—0.6 eV; c) 0.7 eV. Those of the pentavacancies are a a—0.7 eV; b—0.9 eV; c— 1.5 eV.

cies approaches the value of E_{nv}^{B} of a compact cluster having the same number of vacancies (Fig. 7). The binding energies of {100} double layers of vacancies and linear vacancy chains are about 20% lower than the binding energies of compact clusters having the same number of vacancies. The lowest binding energy is exhibited by vacancy monolayers. For all forms of vacancy clusters in α -Fe the binding energy can be described by⁵⁷

where the coefficients α and β are listed in Table III.

If planar vacancy clusters tend to convert into dislocation loops as the number of vacancies in the clusters is increased, ^{57,59,60} at least in fcc crystals, an increase in the dimensions of the most stable compact vacancy clusters results in their conversion into small vacancy pores. An octahedral V_6 vacancy cluster in α -Fe (Fig. 6), for example, may already be regarded as the beginning of a pore.⁵⁸ This conclusion is supported by calculations of the activation energy for the dissociation of a V_6 cluster⁵⁾ into a compact V_5 cluster and a vacancy: 1.46 eV. This value is considerably higher than the dissociation energy of smaller clusters. The next octahedral pore is a compact cluster of 19 vacancies. •

The various forms of vacancy clusters predicted by computer simulations are presently being found by direct observation (by electron microscopy, for the most part) of irradiated metals. It has been found that irregular forms of vacancy clusters and dislocation loops of the vacancy type form in an abrupt manner in cascades of atom-atom collisions,^{61,62} while vacancy pores are usually formed in an annealing process.⁶³

TABLE II. The region of the vacancy-vacancy interaction in α -iron.⁵⁷

Distance between vacancies (the number of the neighborhood)	Number of atomic sites in the inter- action region around one of the vacancies	Interaction energy	
$d \leqslant d_9 \\ d \leqslant d_6 \\ d \leqslant d_4$	136 64 50	$ \geqslant 0.01 \text{ eV } (T = 120 \text{ K}) \geqslant 0.025 \text{ eV } (T = 290 \text{ K}) \geqslant 0.05 \text{ eV } (T = 570 \text{ K}) $	

⁵⁾The "activation energy for the dissociation of a cluster" is the sum of the binding energy of a single vacancy and a cluster and the vacancy migration energy.⁵⁷ An understanding of the actual mechanisms by which less stable cluster forms transform into more stable cluster forms is important, and this question is presently being investigated by computer simulation of defects. It has been established, for example, that in an fcc crystal it is more favorable from the energy standpoint for a vacancy loop to connect vacancies in its own plane than in adjacent planes near the center,^{60,64} with the resulting conversion of the loop into a pore.

Also taking into account the fact that the dissociation energy of a planar cluster is lower than that of a compact cluster, we are led to the suggestion that planar clusters transform into more stable compact clusters through a dissolution of vacancy plates. It has also been hypothesized that there is a dynamic conversion of planar vacancy clusters into three-dimensional clusters⁶⁵ when a cascade of atom-atom collisions passes near a planar vacancy cluster, leaving in its wake a small additional vacancy cluster, which causes the planar cluster to change into a three-dimensional cluster.

Analysis of the structures of interstitial clusters has not revealed the variety of structures exhibited by vacancy clusters. Bullough and Perrin⁶⁶ worked from a dynamic model to study the evolution of the atomic structure of a cluster of interstitial atoms (interstitials, for short) in α -iron. They found that the most stable configuration of three interstitials consisted of three parallel (110) dumbbells in a $\{110\}$ plane. The beginning of a prismatic loop continues to grow in the same plane when the subsequent interstitials are added. The addition of an extra layer of atoms disrupts the regular ... ABAB... alternation of atomic layers of the {110} planes in a bcc lattice, introducing an ... ABAABAB... stacking fault. This stacking fault can be removed by a mutual displacement of the layers of atoms AA, consisting of dumbbells, by a vector (1/2) [001] parallel to the plane of the layer. A prismatic dislocation with a Burgers vector (1/2)[110] bounding a planar cluster of interstitial atoms converts into a slip loop with a Burgers vector (1/2) [110] + (1/2) $[00\overline{1}] = (1/2) [11\overline{1}]$. This loop can undergo a further decrease in energy by rotating from the (110) plane into the (111) plane, again becoming a prismatic loop, but a slip loop in the (110) prism planes. This change in structure sets in (under flexible boundary conditions) when the number of interstitials in the cluster reaches 16. Prismatic loops with



 $(1/2)[11\overline{1})$ Burgers vectors have been observed in irradiated bcc metals.^{67,68}

d) Structure of impurity defects.

Substitutional and interstitial impurity atoms are point defects. Their atomic configurations determine the properties of the solid solution. Insoluble impurities arise during ion implantation and when fast particles cause nuclear reactions. The species resulting from transmutation, in particular, helium, change the properties of the irradiated metal, and this circumstance has stimulated an effort to simulate the corresponding atomic configurations on computers.

It has been established that substitutional impurities create anisotropic atomic displacement fields in their vicinity. The displacement field around helium in a substitutional position in an fcc copper crystal,⁶⁹ for example, is reminiscent of the displacement field around a vacancy: The nearest neighbors are displaced toward the helium, and the second nearest are displaced away from it. The magnitudes of these displacements around helium are considerably smaller than those around a vacancy (see Fig. 2 in Ref. 69).

A substitutional impurity atom does not necessarily occupy a vacant site. A carbon atom in α -iron, for example, does not rest at the center of a vacancy but instead moves away from it along one of the six equivalent (100) directions. Figure 65c in Ref. 27 shows the configuration of substitutional carbon in α -Fe.

Most of the stable configurations of interstitial impurities are mixed dumbbells (Fig. 8). They have also been observed experimentally, by means of the Mössbauer effect, for example.⁷⁰ A mixed dumbbell has different arm lengths (the distances from the lattice site to the impurity atom and to the



FIG. 7. Binding energy of the most stable forms of vacancy clusters in α -iron as a function of the number of vacancies in the cluster.⁵⁸

FIG. 6. Stages in the growth of the most stable configurations of vacancy clusters in α -iron.⁵⁷ a—Growth of V_3 ; b—growth of V_5 ; c—growth of V_8 . The squares are sites at which there are vacancies.

matrix atom are different). The ratio of these lengths, ζ , depends on the particular impurity and the particular matrix crystal. Dederichs et al.⁷¹ have studied the dependence of ζ on the nature of the impurity. They created an artificial impurity atom by displacing the interaction potential (a Morse potential) of the matrix atoms by a certain amount r_0 , thereby creating a new potential for the interaction between an impurity atom and a matrix element.⁶⁾ Negative values of r_0 simulated small impurities, while positive values of r_0 simulated large impurities. It was found that a stable mixed dumbbell does not always form; it forms preferentially when the radius of the impurity is less than that of the matrix atom $(r_0 < 0)$. For large negative values $(|r_0/R| \ge 0.06)$, where R is the distance corresponding to the minimum of the original Morse potential), a mixed dumbbell is unstable. For $r_0/$ R > 0.03, a mixed dumbbell also loses its stability.

The stability of a mixed dumbbell in a bcc iron lattice, with one of the arms of the dumbbell occupied by helium, has been studied by a dynamic model.⁷² A dumbbell of this sort is unstable (Fig. 9). An interstitial matrix atom returns to its site, while helium forms a configuration reminiscent of a static crowdion; this configuration had been predicted by Wilson and Johnson.73 This configuration may be thought of as the limiting case of a dumbbell (cf. Fig. 8). The results of calculations on the formation energies of various configurations of interstitial helium in fcc and bcc metals, on the atomic displacements, and on the migration energies are shown in Tables IV and V. The lowest formation energies for helium were found for the (1, 0, 0) configuration, which was called the "limiting case of a mixed dumbbell" above. An exceptional case is Ni, for which the (1/2, 1/2, 0) configuration is the one most preferable from the energy standpoint. The formation energy of helium in the (1, 0, 1) and (0, 0, 1) configurations is the same in all the bcc metals studied. The formation energies of helium configurations in bcc metals are quite large, in agreement with the poor solubility of helium in

TABLE III. The coefficients α and β in the expression for the binding energy of vacancy clusters in α -iron⁵⁷ ($E_{nv}^{B} = \alpha n - \beta$).

Type of cluster	α, εν	β, eV
Compact {110} double layer {100} double layer Linear chains {110} monolayer {100} monolayer	$\begin{array}{c} 0,79\\ 0,77\\ 0.62\\ 0.6\\ 0.43\\ 0.32\end{array}$	2.853.052.301.301.10

⁶⁾A shift of the Morse potential curve away from the position describing the interaction of matrix atoms by a distance r_0 parallel to the r axis in order to simulate the potential of the interaction between the impurity and the matrix atoms is somewhat contrived and is valid only for rough estimates.



FIG. 8. Structure of a mixed dumbbell in an fcc metal⁷¹ (Morse potential, $r_0/R = -0.06$). 1—Atomic positions for the mixed dumbbell; 2—atomic positions for an "ideal" dumbbell (with an interstitial matrix atom); 3—atomic positions in the ideal lattice.

these metals. The displacement activation energy E^m has been determined from the assumption that the saddle point is at (1/2, 0, 1). The values of E^m are lower in bcc metals than in fcc metals.

e) Interaction of impurities with point defects; structure of mixed clusters.

We already mentioned back in Section 2 that computer simulations not only reveal the equilibrium atomic configurations but also make it possible to "observe" the course of reactions between defects. The simplest reaction of this type—the recombination of Frenkel' pairs— was discussed above. The interaction of impurities with point defects is another field of application of computer simulation.

We would expect that an interstitial impurity would spontaneously recombine with a vacancy and with vacancy clusters, changing their structure, just as an interstitial matrix atom would. This assumption has been tested by a dynamic method for the reaction of interstitial helium with a vacancy⁷⁴ and with divacancies⁵⁶ in a crystal of α -iron. The divacancies consist of two vacancies at lattice sites at distances corresponding to the nearest, second-nearest, and third-nearest neighbors. The zone of the spontaneous interaction of the (He + V, 2V) complex was determined for the vacancy and for each divacancy. Near a vacancy there is a zone of 42 lattice sites at which an incident interstitial helium atom will recombine with the vacancy and adopt a substitutional position. Comparison with the results found for divacancies shows that none of the zones calculated for them is simply the sum of the recombination zones of interstitial



FIG. 9. Breakup of a mixed Fe-He[110] dumbbell in α -iron.⁷² A, He— Initial positions of the atoms; A', He'—positions after the relaxation. The new position of the He atom is at the center of a (100) face.

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helium with a single vacancy. For divacancies, the recombination zones are always smaller than the sum zone for two isolated vacancies (63, 69, and 71 sites vs 84 sites). We see that with increasing density of the divacancy (with increasing binding energy of the divacancy), the zone of spontaneous recombination with an interstitial impurity becoms progressively smaller. The most stable $\langle 100 \rangle$ divacancy corresponds to the smallest recombination zone of the 63 unstable positions of the He atom. Calculations for nickel show⁷⁵ that five He atoms displace one matrix atom from its lattice site and occupy the vacancy which results. Eight He atoms displace two Ni atoms. The formation may be thought of as the beginning of a helium bubble.

The dynamic simulation method, in which the trajectories of all the atoms involved in the reaction are determined in the course of the simulation, has revealed three types of interactions of interstitial helium with a vacancy and a divacancy. Helium moves directly to vacancies at the closest lattice sites, undergoing a single displacement (reaction I). Helium does not ever reach vacancies at more remote sites. It replaces one of the nearest iron atoms, and this iron atom moves to the vacant site (reaction II).

These two types of reactions are also seen in the case of divacancies (Table VI). A reaction peculiar to the recombination of interstitial helium with divacancies is reaction III. It has been observed only in the interaction of helium with a divacancy whose constituent vacancies are at lattice sites at the nearest-neighbor distance; in this type of reaction, the interstitial helium assumes a substitutional position after visiting both vacancies (Fig. 10). The helium atom (the halffilled circle) initially moves toward vacancy 1; after reaching it, it undergoes several large oscillations. In the course of these oscillations, the helium reaches vacancy 2; then it returns to vacancy 1; and it finally stops at vacancy 2, assuming the position of a substitutional impurity.

The binding energies of the (He + 2V) complexes formed after the recombination reaction have been calculated for all these reactions of divacancies with interstitial helium. The results are shown in Table VI, where the complexes in which helium does not recombine with divacancies (the helium is outside the spontaneous-recombination zone) are called "reactions of type IV." It can been concluded from this table that for all complexes formed after recombination the binding energy is sufficiently high (1.93–4.57 eV), while the complexes in which helium remains outside the recombination zone have a low or negative binding energy (from - 0.010 to 0.059 eV).

Several experimental studies^{76,77} suggest that interstitial matrix atoms interact with impurity atoms. In particular, it has been suggested that in cubic metals the capture of an interstitial matrix atom by an impurity gives rise to mixed dumbbells, discussed in the preceding subsection. There is the further possibility of other configurations of complexes consisting of an impurity and an interstitial matrix atom.⁷⁸

Johnson and Lam⁷⁹ have suggested that a bond forms between an impurity (a substitutional impurity) and an interstitial matrix atom in an fcc metal when the impuity occupies one end of a dumbbell or when the dumbbell is at the position of the nearest or second-nearest neighbor of an impurity

TABLE IV. Formation energies (in electron volts) of interstitial helium atoms in fcc metals. The activation energies for a displacement are given in the last column. The numbers in parentheses are the displacements of the nearest neighbors, expressed in units of half the lattice constant.⁷³

-	C	Activation energy for a		
Metal	(1, 0, 0)	(1/2, 1/2, 0)	(1/2, 1/2, 1/2)	displacement of the interstitial helium, eV
Ni Cu Pd Ag	$\begin{array}{c} 4,60 \ (-0,121) \\ 2,03 \ (-0,069) \\ 3.68 \ (-0,071) \\ 1.53 \ (-0,052) \end{array}$	$\begin{array}{c} 4.52 (-0.246) \\ 2.60 (-0.215) \\ 5.42 (-0.182) \\ 2.39 (-0.200) \end{array}$	$\begin{array}{c} 5,39 \ (-0.092) \\ 2,96 \ (-0.074) \\ 5.43 \ (-0.062) \\ 2,60 \ (-0.058) \end{array}$	$0.08 \\ 0.57 \\ 1.74 \\ 0.86$

atom. The binding energies of complexes of this type were estimated by Dederichs *et al.*⁷¹ These calculations confirmed that clusters of this type might form, and they revealed a restriction imposed on their stability by the relative size of the impurity.

The actual reaction by which a substitutional impurity (helium) captures an interstitial matrix atom has been simulated for bcc iron.⁷² For an analysis of the interaction of a dumbbell interstitial with a helium atom in a substitutional position, the helium was put in turn at various positions with respect to the center of the dumbbell interstitial. In the process of the dynamic calculation, a stable (He + i) cluster configuration was established as the energy of the microcrystallite approached a minimum. When the helium reaches the site of the nearest neighbor of the center of the dumbbell, one of its atoms is thus attracted to the helium atom. The helium abandons its position and assumes a substitutional position, occupying the center of the edge of a cube (this configuration was described in the preceding subsection). The interstitial iron atom occupies the site formerly occupied by the helium.

All complexes of a dumbbell with helium at a nearestneighbor site are unstable. Complexes consisting of a dumbbell and helium at a second-nearest-neighbor site with respect to the center of the dumbbell behave in a more complicated way. Capture occurs only when one of the atoms of the dumbbell and the helium atom are separated by less than a lattice constant. Four of the sixth second-nearestneighbor positions are of this type. Here we see evidence of the dependence of the structure of the capture zone on the orientation of the dumbbell interstitial; this dependence was later confirmed for more remote neighbors. As in the case of nearest neighbors, the capture occurs through the attraction of one of the atoms of the dumbbell to the helium, which is displaced from its position and undergoes a transition from a substitutional position to an interstitial position.

When an interstitial atom reaches sites corresponding to the third-nearest and more remote neighbors of the helium atom, the capture occurs only along close-packed directions, and of these directions only along those which lie in the (110) plane of the dumbbell interstitial (Fig. 11). The capture process is quite different in this case. The capture does not result from the direct attraction of one of the dumbbell atoms to the helium. One of the atoms of the dumbbell interstitial replaces its nearest neighbor along the line connecting the center of the dumbbell to the helium atom (the $\langle 111 \rangle$ direction). The displaced nearest neighbor in turn displaces the helium atom, knocking it out of its static-crowdion position on the edge of the cell. A similar chain of replacements, but longer, occurs when the helium is farther from the dumbbell interstitial (out to the fourth-nearest neighbor along the $\langle 111 \rangle$ direction).

In parallel with the analysis of the capture, the binding energy of a cluster consisting of helium and an interstitial atom was determined for various relative positions of the cluster components. The binding energies are positive and approximately the same in magnitude for all positions of the cluster when there is an attraction of the interstitial atoms to the helium atom which terminates in the formation of a static crowdion with helium at the center. For all other configurations the binding energy turned out to be negative.

TABLE V. Formation energies (in electron volts) of interstitial helium atoms in bcc metals. The activation energies for the displacement of interstitial helium (in electron volts) are shown in the last column.⁷³

Coordinates of helium atom	Vanadium	Iron	Molybdenum	Tantalum	Tungsten
$\begin{array}{c} 1,0,1\\0,5,0,1\\0,0,1\\0.75;\ 0.25;\ 1\\0,5;\ 0.5;\ 1\\0,25;\ 0.75;\ 1\\0,75;\ 0.25;\ 0.75\\0.50;\ 0.50;\ 0.50\\0.25;\ 0.75;\ 0.25\end{array}$	$\begin{array}{r} 4.61\\ 4.74\\ 4.61\\ 4.90\\ 5.38\\ 4.90\\ 5.02\\ 5.18\\ 5.02 \end{array}$	5,36 5,53 5,36 5,76 6,28 5,76 5,80 6,16 5,79	$\begin{array}{c} 4.91 \\ 5.14 \\ 4.91 \\ 5.55 \\ 6.52 \\ 5.55 \\ 5.67 \\ 6.56 \\ 5.66 \\ 5.66 \end{array}$	$\begin{array}{r} 4.23 \\ 4.22 \\ 4.23 \\ 4.60 \\ 5.04 \\ 4.60 \\ 4.62 \\ 5.15 \\ 4.61 \end{array}$	5.47 5.71 5.47 6.19 6.32 7.44 6.32
Activation energy for the displacement of interstitial helium (eV)	0,13	0,17	0.23	0.01	0.24

TABLE VI. Characteristics of the reactions of interstitial helium with various divacancies.⁵⁶

Type of divacancy	$E_{2\mathbf{V}}^{\mathbf{B}}, \mathbf{eV}$	E_{2V}^{B} , eV ¹⁷	Size of spontaneous- recombination zone	Type of reaction	$egin{array}{c} \mathbf{E}_{\mathbf{H}\mathbf{C}+2\mathbf{V}}^{\mathbf{B}},\\ \mathbf{eV} \end{array}$
Constituent vacancies at the nearest-neighbor- distance	0.21	0.13	69	II III IV	${}^{4,57-3,23}_{4.58-2,72}_{-0.01}$
Constituent vacancies at the second-nearest neighbor distance	0,47	0,20	63	I II IV	4.48 - 4,18 3.12 - 2,23 -0.04
Constituent vacancies at the third-nearest-neighbor distance	0,10	_	71	I II IV	3.75 - 1.93 3.59 - 2.48 -0.06

The general configuration of the capture zone, if capture is understood as meaning the formation of a complex of an impurity with an interstitial atom with a positive binding energy, is very anisotropic, being stretched out along the (100) and (111) directions. The capture always terminates in the formation of the same (He + i) cluster configuration: The helium goes from a substitutional state to an interstitial state, forming a static crowdion along the (100) direction, while the interstitial matrix atom occupies its lattice site. The capture process is reminiscent of the spontaneous annihilation of a Frenkel' pair. With its small radius, helium forms a displacement field around itself which is qualitatively reminescent of the displacement field around a vacancy. An interstitial atom tends toward this density decrease. A similar behavior of interstitial atoms upon the capture of an impurity should be expected also for other small impurities.

This capture process, in which there is a substantial change in the original configuration of the (He + i) cluster, may be classified as "strong" capture. One consequence of strong capture is a switching of the roles of the interstitial matrix atom and the impurity atom (the helium atom goes to an interstitial position).

Simulation of the course of reactions of impurities with vacancies and interstitial atoms provides important information for constructing a theory for the annealing of defects. This research approach is hindered, however, by the length of the calculations. There is a more active program in simulating the final products of these reactions: the mixed complexes which vacancies and interstitial atoms enter along with impurities.

Andermann and Gehman⁸⁰ have used dynamic simulation to study a large set of xenon-vacancy clusters in copper. Their results are shown in Table VII. The second and third columns contain the number of vacancies (N_V) and the number of xenon atoms (N_{Xe}) in the cluster. Clusters with up to 15 vacancies and up to 12 xenon atoms were studied. The fourth column shows the total formation energy for N_V isolated vacancies and N_{Xe} isolated xenon atoms (in substitutional positions) in the copper lattice. Here $E_V = 1.00$ eV is the vacancy formation energy, $E_{Xe} = 5.67$ eV is the formation energy of substitutional xenon, E_F is the formation energy of a mixed cluster, and E_B/N_{Xe} is the binding energy per xenon atom.

We see from this table that clusters consisting only of xenon atoms without a vacancy are unstable. Also unstable are those mixed clusters in which the ratio of the number of vacancies to the number of xenon atoms, $N_V/N_{\rm Xe}$, is small (see cluster 13, for example). These results can be understood by taking into account the large dimension of xenon in comparison with the copper atoms.

Vacancies stabilize the xenon clusters, i.e., increase the binding energy. This conclusion can be illustrated by com-



FIG. 10. Paths traced out by the atoms during the interaction of an interstitial helium atom with a divacancy (reaction III).⁵⁶ 1—Matrix atom; 2 helium atom; 3—vacancy.

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FI. 11. Chain of substitutions in α -iron upon the cpature of an interstitial matrix atom by a helium atom.⁷² The helium atom is in a $\langle 111 \rangle$ close-packed row at the position of the second-nearest neighbor of the center of the dumbbell interstitial. The motion of the surrounding atoms is not indicated. A, A'—Initial and final positions of one of the atoms of the dumbbell interstitial; B, B'—initial and final positions of an atom in the chain of substitutions; C, C'—initial and final positions of the helium atom (the partially filled circle).

TABLE VII. Energy characteristics of	xenon-vacancy c	lusters in copper. ⁸⁰
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Defect	N _V	N _{Xe}	$N_{\mathbf{V}}E_{\mathbf{V}} + N_{\mathbf{X}\mathbf{e}}E_{\mathbf{X}\mathbf{e}}$	E _F	E _B /N _{Xe}
$ \begin{array}{c} 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 9\\ 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ \end{array} $	$\begin{array}{c} 0\\ 0\\ 0\\ 1\\ 1\\ 1\\ 2\\ 4\\ 6\\ 4\\ 6\\ 4\\ 6\\ 4\\ 0\\ 1\\ 6\\ 7\\ 14\\ 15\\ \end{array}$	$ \begin{array}{c} 1\\ 2\\ 1\\ 2\\ 2\\ 2\\ 2\\ 2\\ 2\\ 4\\ 13\\ 12\\ 13\\ 12\\ 13\\ 12\\ 13\\ 12\\ 13\\ 12\\ 13\\ 12\\ 13\\ 12\\ 13\\ 12\\ 13\\ 12\\ 13\\ 12\\ 12\\ 13\\ 12\\ 12\\ 13\\ 12\\ 12\\ 13\\ 12\\ 12\\ 13\\ 12\\ 12\\ 13\\ 12\\ 12\\ 13\\ 12\\ 12\\ 12\\ 12\\ 12\\ 12\\ 12\\ 12\\ 12\\ 12$	5.67 11.34 11.34 6.67 12.34 12.34 13.34 15.34 15.34 17.34 26.68 73.7 69.0 79.7 75.0 87.7 83.0	$\begin{array}{c} 5,67\\ 12,08\\ 11,34\\ 6,05\\ 10,94\\ 10,96\\ 10,72\\ 10,05\\ 12,08\\ 13,00\\ 22,77\\ 80,9\\ 74,2\\ 75,6\\ 68,8\\ 67,4\\ 60,6\\ \end{array}$	$\begin{array}{c} -0.37\\ 0\\ 0.62\\ 0.70\\ 0.69\\ 1.31\\ 2.65\\ 1.63\\ 2.17\\ 0.98\\ -0.55\\ -0.43\\ 0.32\\ 0.52\\ 1.56\\ 1.87\end{array}$

paring defects 3 and 6, where an unstable di-xenon cluster becomes stable through the attachment of a single vacancy.

The binding energy $E_{\rm B}/N_{\rm Xe}$ is affected by not only the ratio $N_{\rm V}/N_{\rm Xe}$ but also the spatial distribution of the vacancies in the cluster. In cluster 9, for example, both the ratio $N_{\rm V}/N_{\rm Xe}$ and the arrangement of xenon atoms are the same as in cluster 8. The value of $E_{\rm B}/N_{\rm Xe}$ in cluster 9, however, is 1 eV lower because of the different arrangement of vacancies. The spatial arrangement of the vacancies has the effect that for a given value of $N_{\rm V}/N_{\rm Xe}$ the ratio $E_{\rm B}/N_{\rm Xe}$ is large when each vacancy in the cluster interacts with the greatest number of gas atoms.

Argon-vacancy clusters in copper behave in a similar way.⁸¹

In addition to clusters containing xenon and argon, simulation methods have been used to study helium-vacancy clusters in copper,⁶⁹ helium bubbles in fcc metals,⁸² divacancies with helium,⁸⁴ and other mixed formations (see the review by Kirsanov⁸⁴).

f) Defect migration in crystals.

As it moves through a crystal a point defect goes from one stable configuration to another, overcoming the energy barrier between these configurations; this barrier is a saddle point on the potential relief of the crystal. The migration activation energy $E_{\rm m}$ is defined as the difference between the potential energies of the crystal with the defect at the saddle point and in the equilibrium configuration. In the course of the thermal vibrations of the lattice, the atoms constituting the point defect (e.g., those surrounding a vacancy) acquire from time to time a kinetic energy sufficient for one of them to overcome the barrier $E_{\rm m}$. However, it is not yet possible to follow the entire path traced out by the system in the multidimensional configuration space, since the algorithms available for incorporating thermal vibrations in the molecular dynamics model¹⁶ cannot reconstruct a stable temperature regime in the model crystal which would exist for a long time. Such a regime is precisely what is required to simulate the long waiting times characteristic of thermally activated defect migration. The basic thrust in the simulation of migration is thus to determine the structure of the defect and its

energy at the saddle point. The saddle point has to be specified hypothetically in the absence of thermal vibrations by working from arguments regarding the geometry of the defect and the lattice. This circumstance results in some uncertainty in the migration paths which are found. The simulations have to be repeated many times in order ultimately to choose the defect paths which are most favorable from the energy standpoint. Even this laborious approach, however, is contributing substantially to our understanding of the migration of defects.

It has been established, for example, that the migration of a vacancy involves the hop of one of the nearest neighbors of the vacancy to the vacancy. As a result, a new vacancy forms at the former position of the atom which has moved, while the previous vacancy has disappeared.

Divacancies move through fcc and hcp lattices through transitions of one of the atoms which are simultaneously neighbors of both vacancies to the position of one of the vacancies. The motion of divacancies in α -Fe has turned out to be more complicated: Each of the vacancies of the divacancy moves separately, and the motion occurs in two steps. In the first step, one of the vacancies occupies the fourth coordination sphere. In the second step, a stable configuration with a vacancy at another site is established. The energy of this motion is less that the calculated value of $E_{\rm m}$ for a single vacancy (0.68 eV), although not greatly different⁷¹ (0.66 eV for α -Fe).¹⁷

According to calculations by Beeler,⁵⁷ the largest mobile vacancy cluster in bcc α -Fe is a trivacancy, which migrates with an activation energy of 0.66 eV. Larger vacancy clusters must undergo a partial dissociation in order to move through the crystal. For example, it would be advantageous from the energy standpoint for a cluster of four vacancies to dissociate into a single vacancy and a trivacancy in order to move (the activation energy for this dissociation is 1.2 eV in α -Fe).⁵⁷

The process by which interstitial atoms move turns out to be slightly more complicated than for vacancies. Figure 12d shows one version of the process for a dumbbell along

⁷Here and below, we give only isolated numerical values of the activation energy, referring the reader to Ref. 85 for a detailed list for many crystals.



e) With change in configuration

FIG. 12. Mechanisms for the diffusive motion of an interstitial atom in a bcc lattice. 88,89

the [110] direction in a bcc crystal. The original dumbbell along the [110] direction, centered at (000), becomes a dumbbell along the [101] direction, centered at (1/2, 1/2, 1/2) after one hop. The activation energy for this motion is 0.33 eV for α -iron.¹⁷ A [100] dumbbell in an fcc lattice migrates in a similar way (with a change in its orientation).⁸⁶

The activation energy for the rotation of the dumbbell around its center in α -iron (Fig. 12c) is also 0.33 eV (Ref. 17). The motion of a crowdion configuration of an interstitial atom (Fig. 2) in α -Fe along a close-packed direction has the lowest activation energy,¹⁷ 0.04 eV. Several other ways in which an interstitial atom moves in a bcc lattice are shown in Fig. 12.

The process shown in Fig. 12e for the motion of an interstitial atom, accompanied by a change in configuration, is worthy of note. That this type of motion is possible was discovered in a direct simulation of the motion event. The idea underlying this computer simulation can be outlined as follows: The defect configuration of interest is formed in a model crystallite (a witness defect). The crystallite is then "locally heated." The source of this local heating could be, for example, the formation of collapse of an unstable Frenkel' pair near the defect.^{87,90} Enough energy is released to activate the motion of the witness defect. Hopping of a defect accompanied by a change in configuration (a dumbbell interstitial converts into a crowdion) has been observed to be induced in α -iron by the collapse of an unstable Frenkel' pair formed along the $\langle 111 \rangle$ direction (Fig. 13).⁸⁹

Johnson¹⁷ has studied the motion of the most stable diinterstitial in a bcc crystal. He showed that the motion of a pair of this sort is a multistep process involving a partial dissociation of interstitial atoms in a transitional stage. The energy of the motion for α -iron is 0.18 eV.

The motion of mixed dumbbells (consisting of an impu-



FIG. 13. Motion of an interstitial witness atom upon the collapse of an unstable Frenkel' pair in the upper part of the figure.⁸⁷ The new configuration of the displaced interstitial atom (a static crowdion) is shown separately at the left.

rity and a matrix atom) turns out to be more complicated than the motion of an interstitial matrix atom. In addition to a migration event similar to the motion of a matrix dumbbell, two unusual processes are predicted: caging and looping.⁷⁹ Caging results from the easy migration of the impurity along symmetric equivalent positions in a bounded configuration. Figure 14a shows an example of such positions, which form a "cage." An interstitial looping (with a low activation energy) around an impurity (Fig. 14b) results in a reversal of the orientation of a mixed dumbbell.

Ingle and Crocker⁹¹ have observed an effect of an external stress on defect migration. They studied the influence of a uniaxial stress on the binding energy of a divacancy, E_{2V}^{B} , in bcc crystals (α -Fe, Mo, W). They found that E_{2V}^{B} increases or decreases, depending on the direction of the applied stress and the orientation of the divacancy. The change in the cluster binding energy involves a change in the migration, which is either facilitated or hindered.

4. DISLOCATION CORES AND INTERACTIONS OF DISLOCATIONS WITH POINT DEFECTS

The original purpose of the computer calculations on dislocation cores in various crystals was to refine the semiphenomenological picture of the fine structure of such cores.



FIG. 14. a—Caging⁷⁹ (the positions occupied by the mixed dumbbell during easy migration of an impurity in the "cage" in an fcc crystal are shown; a filled circle represents an impurity atom, while an open circle represents a matrix atom); b—looping of an impurity in an fcc crystal^{79,71} (shown in succession are the breakup of the mixed dumbbell and the hop of a matrix atom to an adjacent site, the formation of a new dumbbell interstitial, the circumvention of the unit cell by an interstitial matrix atom and its return to the impurity from the other direction; the large circles represent matrix atoms, while the small circle represents an impurity atom).

Details in this picture were subsequently filled in and were found to have a substantial influence on the course of plastic deformation of crystals with bcc, hcp, and other lattices.

In the semiphenomenological model of a core one considers the splitting of the complete dislocation, with Burgers vector **b**, into *n* dislocation partials with Burgers vectors \mathbf{b}'_{i} satisfying $\mathbf{b} = \Sigma^n \mathbf{b}'_i$. Between the dislocation partials there are strips of stacking faults with a surface energy γ (in general, this surface energy is different for different strips; more on this below). With $\gamma \approx 10 \text{ mJ/m}^2$, as in several alloys, the splitting is pronounced; the width (l) of the strips is several nanometers; and the strips can be resolved quite well in an ordinary electron microscope. With γ of the order of hundreds of millijoules per square meter, however, the width l does not exceed a few atomic spacings, and it would be more proper to speak of a complex structure of a dislocation core. rather than a splitting. Only recently has this structure become observable in high-resolution electron microscopes, and many details remain unexplained. For example, we do not understand the structural changes of the core which occur during the slip of a dislocation and which determine the Peierls stress τ^{P} , at which a straight dislocation starts to move.8)

Computer simulation can reveal such details if one assigns the atoms at the boundary of the microcrystallite containing the dislocation displacements which correspond to the application of a tangential stress τ to the crystal.

Another purpose of computer simulation is to calculate and compare the various configurations of the core and to identify the atomic mechanisms for the conversion of one configuration into another, in particular, at a moving dislocation and in crystals with a complex unit cell.

Since a dislocation is a defect of macroscopic size in one dimension, calculations regarding the structure of a dislocation core are possible in practice only for those orientations t of the dislocation line for which the period over which the crystal structure repeats itself along t is no more than a few times the distance between adjacent planes. For edge, screw, 60°, and certain other of the most important orientations, this condition is satisfied. Slight deviations from these orientations are induced by kinks. Their effective width W increases with decreasing $\tau^{\rm P}$. For fcc and alkali halide crystals, W is of the order of a few tens of atomic spacings, and the corresponding calculations which have been carried out on the atomic structure of kinks are unreliable. In bcc crystals, W is lower, and is contained in a calculation cell with several thousand atoms which can be handled by modern computers

The simplest characteristics of the core of an unsplit dislocation which are found by computer simulation are the core radius r_c and the core energy E_c ; this energy is calculated over the repetition period of the structure along the dislocation line, which is equal to the Burgers vector for a screw dislocation. To calculate r_c and E_c one computes the energy of the crystal with the dislocation as a function of the radius

R of a cylinder whose axis coincides with the axis of the dislocation. On a plot of $E |\ln R|$ there is a large scatter in the points at $R \leq 2b$, but at some R_c the points begin to conform well to a straight line which corresponds to the expression $E = Kb^3 \ln[R/r_c]$ from elastic theory, where we would have $K = G/[4\pi(1-\nu)]$ for an edge dislocation in an isotropic medium. Agreement of the value of K found through the computer simulation with the value found from elastic theory is taken as evidence that the interatomic potential has been chosen correctly. The value of R_c is taken to be the core radius r_c , while the core energy is taken to be $E(r_c)$. Since there is some arbitrariness in the definition of r_c , the values given below for r_c and E_c should be regarded as simply illustrative. There is a method for determining τ^P which can be used without modification for crystals of arbitrary symmetry.

without modification for crystals of arbitrary symmetry. The atoms at the boundary of the microcrystallite are assigned displacements which correspond to an elastic strain $\varepsilon = \tau/2G$ in the crystal, caused by the application of a tangential stress τ parallel to the slip plane. This stress is increased in steps, and at each τ_i the equilibrium core configuration is found. At some critical $\tau_i = \tau_c$ the core becomes unstable; the dislocation is displaced a distance equal to the period (a) of the Peierls relief; and the original core structure is reproduced. The shear strain decreases (relaxes). If the tangential displacements at the boundary are held constant, the core shifts to the next groove of the Peierls relief, and so forth, until it reaches a lateral face in the microcrystallite. The particular stress at which the core becomes unstable is taken to be the Peierls stress⁹ τ^{P} .

a) fcc crystals.

The first calculations⁹² on the core of an edge dislocation in copper, carried out by a variational method with a Morse potential, confirmed the concept of a splitting of a dislocation. As expected, the width of the stacking-fault strip was found to depend strongly on the particular choice of interatomic potential and also on the boundary conditions (the size of the microcrystallite).⁹³

If the energy of the stacking fault, γ , is not used as an adjustable parameter in constructing the potential, the lattice statics method⁹⁴ in which calculations are carried out with the interatomic potentials of Ref. 32 yields stackingfault widths which agree with the experimental data for screw dislocations in Al, Cu, and Ag. This method has been used to calculate the positions of the atoms for Al for the case in which the axis of the screw dislocation, (a/2) [110], lies in the z = a/2 plane (A) and in the parallel plane z = a/4 (B). In case B the energy of the core is slightly lower, and the core is slightly split $(l \approx a)$ in the (001) plane. In case A, we have $l \approx 3a$, and the stacking fault is in the {111} plane. Calculations were carried out only for case B for Cu and Ag; the dislocation was in the {111} plane. For Cu the calculations

⁸⁾At a nonzero temperature, a dislocation begins to move at a lower stress through the nucleation of kink pairs. Nevertheless, π^{P} is an important characteristic of a dislocation, since it determines the probability for the thermal-fluctuation nucleation of a kink pair.

⁹⁾A less accurate method for determining $\tau^{\rm P}$ is to calculate the core energy U in various relaxed configurations differing in the specified relative displacement Δx of two selected atomic rows on different sides of the slip plane; Δx is varied from 0 to a. The maximum energy difference $U(\Delta x) - U(0)$ is adopted as the work performed by the Peierls forces, $\tau^{\rm P} b \Delta x$.

yielded $l \approx 3a$, while for Ag they yielded $l \approx 8a$, and dislocation partials were clearly separated.

b) bcc crystals.

The first detailed report⁹⁵ of structural calculations on the core of an edge dislocation with a Burgers vector (a/2) $\langle 111 \rangle$ in the $\{110\}$ plane in iron, carried out by a variational method, gave $E_c = 2.7$ eV as the core energy over the structural repetition period (six $\{112\}$ atomic planes) and gave $\tau^P = 0.0066$ G as the Peierls stress. The dislocation was essentially unsplit, and the core radius was $\tau_c = 0.3$ -0.5 nm.

These calculations were pursued in Refs. 96–98, among others, where one particular goal was to test the possibility of the splitting of a nonscrew dislocation with emergence from the original slip plane.

Gehlen et al.96 carried out molecular-dynamics calculations on the structure of the core of an edge dislocation with a Burgers vector $\mathbf{a}(100)$, which is formed upon the coalescence of two (a/2) (111) dislocations in intersecting slip planes and which may be regarded as the beginning of a microcrack. Johnson's potentials¹⁷ I and II for iron were used along with rigid boundary conditions; the displacements of the atoms at the boundary of the microcrystallite were calculated from isotropic elastic theory. Potential II led to a slightly better agreement of the energies U [the slope of the $U(\ln r)$ curve at $r > r_c$] calculated from the elastic theory and in terms of binary interatomic interactions. In the determination of the constants of potential II from the elastic constants, no correction is made for the conduction electrons. The slip plane of the dislocation is noticeably curved in the core.

De Hosson and Sleeswyk⁹⁸ studied the structure of the core of an $(a/2) \langle 111 \rangle$ edge dislocation in the $\{110\}$ plane in V, W, Mo, and Fe, using the composite polynomial potential of Johnson and Wilson⁹⁹ and rigid boundary conditions corresponding to the anisotropic elastic theory and Vineyard's dynamic method. Incorporating the elastic anisotropy leads to a significant displacement (up to $0.07a_0$) of the atoms of the core along the $\langle 112 \rangle$ dislocation axis. The relative displacements of the atoms along the direction of the Burgers vector vary smoothly with distance from the dislocation axis; only in V is there a hint of the formation of a stacking-fault strip, but this is a consequence of the particular potential $\varphi(r)$. Various modes of the splitting of an edge dislocation have been discussed in the literature.^{100,101} The results of Ref. 98 at best hint at such a splitting.

A mixed dislocation with a Burgers vector $(a/2) \langle 111 \rangle$ in the $\langle 110 \rangle$ orientation in W was the subject of calculations in Ref. 102 with the Beeler potential.¹⁰³ The values $r_c = 0.4$ nm and $E_c = 3.0-3.5$ eV were found.

When d electrons and the interaction of atoms in the second coordination sphere are taken into account in a determination of the total energy of a crystal with a defect, the structure of the core of an edge dislocation is changed considerably.⁴² Depending on the ratio of the screening constants q and p in (24), the distribution of the Burgers vector in the (112) slip plane, b'(x), has either one or two humps. In the case of two humps, they are at a distance of about $3a_0$, and

the full width of the dislocation at half the height of the hump, b', is about $5.5a_0$ (for q/p = 0.28), indicating a rather clear splitting. In the case of the single hump, the width of the core is about $5a_0$ (at q/p = 0.20). In the (100) slip plane, the distribution b'(x) is sharper, with a hump about $1.5a_0$ wide; at q/p = 0.28, the main b'(x) peak is flanked by two smaller symmetric peaks, while at q/p = 0.20 the wings of the main peak are smooth.

The core of a screw dislocation in a bcc lattice has a considerably more complicated structure. Computer simulation has revealed the particular conditions under which the splittings suggested by various authors actually occur (the subject is reviewed by Vitek¹⁰¹). It turns out that the results depend strongly on the particular potential which is chosen, ¹⁰⁴ especially the cutoff radius r_0 . At small values of r_0 (between the radii of the second and third coordination spheres, r_2 and r_3), the splitting is very pronounced, while at larger values of r_0 the slitting is considerably weaker.^{104,105}

Suzuki¹⁰⁶ has proposed a simplified method for describing the atomic structure of the core of a screw dislocation. He introduced a potential to describe the interaction between two rigid atomic rows which run parallel to the OZdislocation axis, which are at the distance r_1 characteristic of the defect-free lattice, and which have a relative displacement along the OZ axis equal to a fraction $\xi = (z_i - z_j)/b$ of the structural repetition period (b) along OZ:

$$\Phi_{ij} = A \cos 2\pi\xi, \quad A = \frac{b^2 \left(c_{11} - c_{12} + c_{44}\right)}{6 \sqrt{3} \pi^2}.$$
 (27)

Displacements of the atoms normal to the dislocation axis are ignored. This method has proved useful for simulating the motion of a dislocation under the influence of an external stress and for determining τ^{P} , but it does not bring out the fine details of the core structure.

The results of these calculations are conveniently displayed as a diagram of differential displacements¹⁰⁷ (Fig. 15), on which the circles on the projection onto the (111) plane represent [111] atomic rows, while the arrows between them represent the relative displacements of adjacent rows along the dislocation axis. The longest arrow represents a displacement of b/3; if the displacement is greater than this, a second arrow is added to indicate the additional displacement.

Calculations using a model of binary interactions of the individual atoms are more laborious but do not suffer from the disadvantages of the method of Ref. 106. The results found by this approach may be summarized as follows¹⁰⁸ (Fig. 15): The stable core structure is degenerate, corresponding to two configurations (Fig. 15a) with identical energies. For certain types of potentials representing the interaction between rows, Φ_{ij} , and for certain values of the parameters of this potential (four types of potentials were studied in Ref. 108), there are the further possibilities of a nondegenerate structure (Fig. 15b) and a triply degenerate structure, a "split core" (Fig. 15c), in which the dislocation axis nearly coincides with one of the rows.

An external tangential stress in the $\{110\}$ plane causes a dislocation with a degenerate core (Fig. 15a) to move in a zigzag fashion, switching from one configuration to another; the resultant slip direction is the $\{112\}$ plane¹⁰⁹ (the 1 \rightarrow 3



FIG. 15. Core of a screw dislocation in a bcc lattice.¹⁰⁸ a—Doubly degenerate stable core; b—nondegenerate core; c—triply degenerate metastable core.

direction in Fig. 16). When the stress acts in the $\{112\}$ plane in a twinning direction, there is a sequence of structural changes as shown in Fig. 17; if the stress instead acts in an antitwinning direction, we have the situation in Fig. 18. A nondegenerate configuration (Fig. 15b) moves one atomic spacing in one of the $\{110\}$ planes, passing through a degenerate configuration¹⁰⁸ (Fig. 15c).

When the energy of the d electrons is taken into account by the method of Ref. 38, and when the interaction of second nearest neighbors is taken into account, we again find changes in the core structure of an (a/2) (111) screw dislocation. As has been shown¹¹⁰ for the cases of Nb, α -Fe, and W, the resulting configuration can be symmetric (nondegenerate) or slightly split and triply degenerate, depending on where the center of the dislocation is placed before the relaxation (Figs. 15a and 15b). If the initial configuration is a split star of three (a/6) (111) dislocation partials, then its relaxation leads to the structure in Fig. 15a, while an initial planar configuration (a/3) (111) + (a/6) (111) leads to the structure in Fig. 15b. Although each configuration can be found without considering the d-electron energy, the energy of the configuration in Fig. 15b turns out to be lower when the d electrons are taken into account (Table VIII). If the interaction of only the nearest neighbors is taken into account, the relaxation leads to configurations with a much more pronounced splitting. Masuda and Sato¹¹⁰ conclude that the split core of a screw dislocation is simply an artifact, in



FIG. 16. Successive configurations of the core of a screw dislocation as it moves under the influence of a tangential stress in the $\{110\}$ plane.¹⁰⁹

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agreement with the conclusion reached by Vitek.¹⁰⁴ In order to explain the low mobility of screw dislocations in the bcc lattice in this case, it is necessary to recompute the Peierls stress and the structure of the kink with allowance for d electrons.

A structure similar to those which we have been discussing is exhibited by the core of a twinning screw dislocation in W in a ($\overline{112}$) twinning plane.¹¹¹ There is a dilatation region in the dislocation core to which interstitial atoms are attracted. These atoms are bound to the dislocation with an energy of 0.15 eV. Boïko *et al.*¹¹¹ proposed a graphic method for displaying the energy distribution in extended defects: Each atom is enclosed by a circle whose radius is proportional to the energy of the atom as calculated from the binaryinteraction formula (se also Ref. 112).

c) hcp crystals.

It may be assumed that one of the reasons why the mechanical properties of different hcp metals differ so greatly is the structure of the dislocation cores in these metals, which is determined by the particular interatomic interactions. As yet we do not have interatomic potentials to describe these distinctive features of the interactions, so that the calculations which have been carried out have been based on the Lennard-Jones potential

$$\varphi(r) = \varepsilon_0 \left[\left(\frac{d}{r} \right)^{12} - 2 \left(\frac{d}{r} \right)^6 \right], \qquad (28)$$

where $d \approx a$, a is the atomic spacing in the basis plane, ε_0 is adjusted to fit (for example) the experimental values of the



FIG. 17. Successive configurations of the core of a screw disloation as it moves under the influence of a tangential stress in the $\{112\}$ plane in the twinning direction.¹⁰⁹



FIG. 18. The same as in Fig. 17, but the force $\tau \mathbf{b}$ is now acting in the antitwinning direction.¹⁰⁹

elastic constants, and the potential is cut off between the fifth and sixth (LJ5) or between the sixth and seventh (LJ6) coordination spheres. A suitable polynomial is of course used to provide a smooth transition from potential (28) to zero. The ratio of axes c/a is found to be 1.6260 and 1.6312, respectively.

The most common dislocations in hcp crystals have a Burgers vector $b = (a/3) \langle 11\overline{2}0 \rangle$; these dislocations can slip in the {0001} basis plane or in the {1010} prismatic plane. The structures of the cores of these dislocations in the edge and screw orientations have been studied by Bacon and Martin¹¹³ with the LJ5 and LJ6 potentials. The results have been displayed as differential-displacement diagrams, as curves of the relative displacements $\Delta u(x)$ of the atomic rows on different sides of the slip plane, and as curves of the density of the Burgers vector, $\rho_x(x) = d\Delta u/dx$ (the x axis runs along [2110], the y along [0110], and the z axis along [0001]).

The core of an edge dislocation in the prismatic plane is wider than predicted by the elastic theory, but there is no splitting into separate partials. A screw dislocation in the basis plane is split; with the LJ5 potential, its width is $W \approx 3a$, and with LJ6 it is $W \approx 10a$ (Fig. 19). An edge dislocation in the basis plane with the LJ5 potential gives us W = (7-8)a, and each dislocation partial on the $\rho(x)$ curve has a peak split in two (Fig. 20).

Under an increasing stress $\tau = 2G\varepsilon$, the core structure initially becomes greatly deformed (in contrast with the situation in bcc crystals), and this deformation continues until the dislocation has moved a distance *a* at the critical value τ^{P} . The values of ε^{P} corresponding to τ^{P} are listed in Table IX. Dislocations in the prismatic plane are also left unsplit by the stress τ . The way in which the core of a screw dislocation split in the basis plane is deformed by a tangential stress in the prismatic plane does not involve the motion of two dislocation partials toward each other (Fig. 19); instead, the Burgers vector of one of the partials increases at the expense

TABLE XIII.	Energy	of a	screw	dislocation
per atomic pla	ne, eV.			

Configuration in Fig. 15	Fig. 15, a	Fig. 15, b			
Nb a-Fe a-Fe W	0.3338 0,5342 0,5800*) 1,3380	0.2790 0,5014 0.5810*) 1.2530			
*The d-electron energy is ignored					

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of the Burgers vector of the other, and then the dislocation slips in the prismatic plane (Fig. 21).

The potentials in (28) have also been used for calculations for the cores of dislocations with a Burgers vector $b = (a/3) \langle \overline{11}23 \rangle$, which can slip in $\{11\overline{2}2\}$ and $\{10\overline{1}1\}$ pyramidal planes. The core of an edge dislocation in the $\{11\overline{2}2\}$ plane can have two structures. One of them (I) can be described as consisting of two $(11\overline{2}2)$ and $(11\overline{2}1)$ twins to the right and left of the center of the dislocation¹¹⁴ (Fig. 22a). The other¹¹⁵ (II) consists of two dislocation partials with Burgers vectors b/2 which are connected by a stacking fault. The dislocation at the left is related to two $(11\overline{2}2)$ and $[11\overline{2}1)$ twins, while that on the right is related to a single (1122) twin (Fig. 22b). Depending on the direction of the force τb , an applied stress τ may have either of two consequences: Either a core of structure I acquires a structure II, and the split dislocation splits, or a twin is formed from both configurations.¹¹⁵ A given dislocation may thus undergo either slip or twinning, depending on the deformation conditions.

A screw dislocation splits into two partials with Burgers vectors $(a/6)\langle \overline{1123} \rangle$; the stacking fault may consist



FIG. 19. Screw dislocation in the basis plane of an hcp lattice.¹¹³ a— Projections of the atoms onto the (2110) plane, LJ5 potential; b—the dispslacements Δu_x and Δu_x in units of *a*; c—the Burgers-vector densities $\rho_x(x)$ and $\rho_x(x)$.



FIG. 20. Core of an edge dislocation in the basis plane with the LJ5 potential.¹¹³ a—Projection of the atoms onto the $(0\bar{1}10)$ plane; b—the displacements Δu_x and Δu_x ; c—the Burgers-vector densities $\rho_{x(x)}$ and ρ_{ex}

of several abutting bands lying alternately in $\{10\overline{1}1\}$ and $\{11\overline{2}2\}$ planes, with nearly equal energies γ (Fig. 23).¹¹⁶ The zonal twinning dislocations which have been discussed in the literature are not found.

d) Ordered alloys.

The translation vector in an ordered alloy is known to be larger than in the corresponding "disordered" lattice. In



FIG. 21. Effect of an increase in the shear strain in a prismatic plane on the displacements 4. (in units of .) and the Burgers-vector density ρ for a screw dislocation in a crystal simulated with the LJ5 potential.¹¹⁴

TABLE IX. Critical stains ε^{P} corresponding to the Peierls stresses τ^{F} (Ref. 113).

Potential	Edge dislocation in		Screw di in basis slipping	slocation plane, in
	Prismatic plane	Basis plane	Prismatic plane	Basis plane
LJ5 LJ6	0,022 0,014	0,011	0.053 0.092	0,015 0.016

particular, in the fcc structure L1₂, typical of many $A^{III}B$ alloys, e.g., Cu₃Au, the Burgers vector of a perfect dislocation (also called a "superdislocation" is 2b, where b is the atomic spacing. A dislocation of this type would tend to split in the {111} slip plane into two dislocation partials, separated by bands with the structure of an intrinsic stacking fault with an energy γ or the structure of an antiphase boundary with an energy ξ . The splitting is described by the reaction

$$a\,[\overline{1}01] \rightarrow \frac{a}{3}\,[\overline{2}11] + \frac{a}{3}\,[\overline{1}\,\overline{1}2],\tag{29}$$

or

$$a\,\overline{[101]} \rightarrow \frac{a}{2}\,\overline{[101]} + \frac{a}{2}\,\overline{[101]} \pm a\,\frac{\chi\sigma}{6}\,\overline{[121]}. \tag{30}$$

In case (30), each of the constituent $a\langle 110\rangle$ dislocations may in turn undergo a crystallographic splitting into two dislocation partials in the same plane; alternatively, if the dislocations are screw dislocations, then this splitting may occur in one of the intersecting {111} transverse-slip planes. There may be a tendency for a lowering of the energy of the antiphase boundary through a displacement $\chi_a \sqrt{6}$ along the $[\bar{1}2\bar{1}]$ direction; the magnitude of this displacement depends on the particular interatomic potentials φ_{AA} and φ_{BB} , as is shown by the last terms in (30).

As a result, the configurations shown schematically in Fig. 24 (C and D arise for various interatomic potential functions φ_{AA} and φ_{BB} (in the approximation of the nearest-neighbor interactions). The notation of these configurations is that of Ref. 117.

If a perfect dislocation is split in a (100) slip plane, the dislocation partials can be separated only by an antiphase boundary, since the energy ξ_{100} (without a stacking fault) in this plane is significantly lower than the energy of a stacking fault, γ_{100} . A crystallographic splitting of each of the (a/2) (101) dislocation partials can occur in the $(1\bar{1}1)$ (F_1) plane and the (111) (F_2) plane. Calculations with a smoother potential spread the core of the screw dislocation partial over both planes, $(1\bar{1}1)$ and (111) (G_1 , G_2).

The type of splitting determines the mobility of the dislocations and, in particular, the mechanism for the transverse slip of the screw dislocation. This slip is responsible for the thermal anomalies of the yield point and other unique mechanical properties of ordered alloys with the $L1_2$ structure.

Kozlov *et al.*¹¹⁸ carried out the first calculations on the core structure and Peierls relief of an unsplit partial screw dislocation with a $\langle 110 \rangle$ Burgers vector in the Cu₃Au alloy. The second dislocation of the pair was not simulated because



of the limited computer memory, and the antiphase boundary went outside the calculation cell.

In an effort to determine the conditions under which the various types of splittings occur, calculations have been carried out on the equilibrium structures of the core of an $a\langle 110 \rangle$ screw dislocation in and Ll₂ structure in the free state and under a tangential stress τ , with several potentials φ_{AA} and φ_{AB} ; the calculations have yielded various values of the energies γ and ξ (Ref. 119). It was found that an intrinsic stacking fault in the {111} plane and an antiphase boundary in the {100} plane are stable regardless of the potential, so that a perfect dislocation with an $a\langle 101 \rangle$ Burgers vector always splits. A complex stacking fault (a super-position of a stacking fault and an antiphase boundary) and an antiphase boundary in the {111} plane may be unstable, causing a "spreading" of the core and various types of splittings (Fig. 24).

Under the influence of a stress τ , the slipping configurations begin moving comparatively easily, and the critical stress for motion to be initiated is essentially $\tau_c = \gamma'/b_P$, where b_P is the projection of the Burgers vector of the dislocation partial onto the corresponding $\langle 110 \rangle$ direction, and γ' is the energy of the stacking fault or antiphase boundary. For sessile configurations, τ_c is considerably larger, and it can be found by studying the behavior of simply one dislocation partial, with the second being taken into account only through its elastic field. All the configurations shown in Fig. 24 have been studied. Structural changes of sessile configurations into various slipping configurations begin only at $\tau = 0.03-0.04$ G.

The sessile configurations C1, D3, F, and G in Fig. 24 behave in different ways. In particular, the splitting corre-



FIG. 23. Core configuration of screw dislocations spread over $(10\overline{1}1)$, $(1\overline{1}22)$, and $(01\overline{1}1)$ planes.¹¹⁶ Projection onto the $(\overline{1}\overline{1}23)$ plane. The arrows dhow the relative displacements of the atomic rows of only oe species, indicated by the squares.

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FIG. 22. a—Projection of the core configuration I of an edge dislocation onto the (1100) plane¹¹⁵ (two twinned regions are shown; the order of the alternation of levels which the atoms assume corresponds to the sequence square; circle; hexagon; rhombus); b—projection of the core configuration II of an edge dislocation onto the (1100) plane.¹¹⁵

sponding to (30) leads to an anomalous increase in the deforming stress σ at elevated temperatures, while the splitting corresponding to (29) leads to an increase in σ at low temperatures (as in bcc metals). Th effect of impurities has been discussed; they promote the transition of the Ll₂ structure into the DO₁₉ hexagonal structure or the DO₂₂ cubic structure. The latter intensify the thermal anomalies in σ .

Takeuchi¹²⁰ has carried out calculations on the motion of a screw perfect dislocation with an $a\langle 111 \rangle$ Burgers vector in ordered alloys with a bcc lattice (B2) under the influence of a stress τ , in the approximation of rigid atomic rows. Two potentials for the interaction btween rows were used:

$$\Phi_{I} = \Phi_{0} \left(\cos 2\pi \xi - \alpha \cos 4\pi \xi + \frac{1-\alpha}{2} \right)$$
(31)

and $\Phi_{\rm II}$, formed by joining five parabolic arcs. The constants Φ_0, α , and those in $\Phi_{\rm II}$ determine the energies γ and $\xi; \xi$ and α are related by¹²¹

$$\xi_{100} = \frac{\sqrt{3} \, Gb}{\sqrt{2} \, \pi^2 \, (1 - 4\alpha)} \,. \tag{32}$$

If $\xi_{100} > 0.006 \ Gb$, the slip occurs more easily along $\{110\}$ planes, while if $\xi_{110} < 0.006 \ Gb$, it occurs more easily along $\{112\}$ planes. The deforming stress σ has been calculated as a function of the angle (χ) between the plane of the maximum shear stress and the nearest $\{110\}$ plane. Most of the experimental data on several alloys with B2 structure agree with the calculated results.

So far, we have no corresponding results for dislocations in more complicated metal structures.

e) Interaction of dislocations with point defects.

The interactions of dislocations with point defects are the governing interactions in aging, the formation of Guinier-Preston zones and precipitates at dislocations, radiationinduced growth and swelling, and radiation-induced creep. These interactions are important over distances of the order of the interatomic distances, and the corresponding calculations must be carried out at the atomic level.¹²²⁻¹²⁷

FIG. 24. Models of the superstructural and crystallographic splittings of a dislocation with *..(110) in the $L1_2$ lattice.

As an example we single out the study by Ingle and Crocker, 126 of the interaction between vacancies and a (1/2) (111) {110} edge dislocation in γ -iron, carried out by a variational method. The dimension of the calculation cell along the normal to the $(1\overline{1}0)$ slip plane was equal to 14 times the distance between planes, that along the [111] Burgers vector was equal to 36 times the distance between planes, and periodic boundary conditions at 6 times the distance between planes (the structural repetition period) or 18 times this distance were imposed along the $[11\overline{2}]$ dislocation line. What was actually simulated was thus not the interaction of a dislocation with a single vacancy but the interaction of a dislocation with a continuous chain of vacancies (6) or a thinnedout chain (18). The two defects (the dislocation and the vacancy) were introduced simultaneously in the model crystallite in most of the calculation versions, and then an energy-minimization procedure was carried out. Unstable configurations were observed. These instabilities were monitored by another method, involving an initial calculation of the structure of the dislocation, followed by the introduction of a second defect and a second minimization. In addition, the interatomic potential was varied.

The most important characteristic—the interaction energy of the vacancy and the dislocation— was calculated by determining various energies which were found directly in the course of the simulation. Denoting by E^{P} the energy of the perfect crystal and E^{P+D} the energy of the crystallite in which a dislocation has been introduced, we can write the energy associated with the dislocation as $E^{D} = E^{P+D} - E^{P}$. Correspondingly, the energy associated with the vacancy is $E^{V} = E^{P+V} - E^{P}$, where E^{P+V} is the energy of a crystallite containing a single vacancy. Denoting by E^{P+D+V} the energy of a crystallite containing both a dislocation and a vacancy, we can write the energy of the interaction between the two defects as

$$E_{\mathbf{I}}^{\mathbf{D}\mathbf{V}} = E^{\mathbf{P}+\mathbf{D}+\mathbf{V}} - E^{\mathbf{P}} - E^{\mathbf{D}} - E^{\mathbf{V}}$$
$$= E^{\mathbf{P}+\mathbf{D}+\mathbf{V}} + E^{\mathbf{P}} - E^{\mathbf{P}+\mathbf{D}} - E^{\mathbf{P}+\mathbf{V}}.$$
(33)

Figure 25 summarizes the results calculated on the energy of the interaction between a vacancy and a $(1/2)(111){110}$ dislocation. Shown here is the projection onto the $\{112\}$ plane of the relaxed dislocation structure. Only the left half of the projection is shown, since the structure is symmetric with respect to the (111) plane, which passes through the dislocation line. The points are the positions of atoms, while the numbers are the dislocation-vacancy bind-

$$\begin{array}{c} (110) \\ 110$$

FIG. 25. Interaction between a vacancy and a (1/2)(111)(110) edge dislocation in α -iron.¹²⁶

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ing energies $E_{\rm B}^{\rm DV}$ (= $-E_{\rm I}^{\rm DV}$), in electron volts. The arrangement of the numbers corresponds to the atomic sites at which there are vacancies. All these numbers are positive, indicating that the interaction is attractive. In the compression region above the slip plane the binding energy is higher than in the rarefaction region below the slip plane. This result agrees with predictions based on a size effect in elastic theory (see Ref. 128, for example), according to which a vacancy would be expected to relieve a stress field above the slip plane. The fact that the binding energy does not change sign below the slip plane, however, indicates that something other than the size effect must also be taken into account.

Several (nine) of the atomic sites in Fig. 25 are shown as open circles. When a vacancy is put in one of these sites, the center of the dislocation core moves a distance (specified by the number above the circle, in units of the distance between planes) in the slip plane. Positive numbers correspond to motion in the direction opposite the vacancy. This effect, however, is the result of the periodic boundary conditions, and it describes the interaction of a dislocation not with a single vacancy but with a chain of vacancies.

f) Migration of point defects along dislocations.

The simulation of defect migration along dislocation cores has led to a refinement of the mechanism for the accelerated "pipe" diffusion which has been observed experimentally on several occasions.¹²⁹ Zhuravlev and Fidel'man^{130,131} used a dynamic method with artificial energy dissipation to study the hopping of vacancies in the cores of [100](010), (1/ 2)[111](110), and (1/2)[111](112) edge dislocations in bcc metals (iron, molybdenum, and tungsten) and of (1/ 2)[110](111) edge dislocations in fcc metals (aluminum, silver, gold, copper, and nickel). A single vacancy was produced by removing one atom from the edge of the extra plane of an unsplit perfect or isolated partial dislocation (bounding a stacking fault). The migration of the vacancy was simulated by the discrete motion (10-20 steps) of one of the neighboring atoms in the direction of the vacancy. In each step in this motion, the atomic structure in the calculation cell underwent relaxation, and the excess energy of the system associated with the current position of the atom which had moved was calculated. In this manner they determined the energy profile of the migration path, on which there was a saddle point, and they thus determined the activation energy for migration of the vacancy along the line of an edge dislocation. In a similar way, they determined the activation energy for motion of the vacancy at other points in the dislocation cores and in the volume. The results of these calculations were compared.

It was found that the formation energy and migration energy of vacancies in dislocation cores are 30-40% lower than the values calculated for the volume of the metal in both fcc and bcc lattices. The region of accelerated diffusion has a radius of one or two Burgers vectors, judging from the activation energy. The results of these calculations, which indicate that an accelerated migration of vacancies may occur along dislocations, have been confirmed by other investigators.

Miller et al.¹³² used a variational procedure to study diffusion along the cores of edge dislocations with a Burgers vector (1/2)[111] in the (110) and (112) slip planes (cases a and b, respectively) in bcc metals (iron and molybdenum). The activiation energy for pipe self-diffusion, Q_p , was calculated for the migration of the vacancies along the most advantageous path. They found $Q_p^{(a)} = 1.76 \text{ eV}$ and $Q_p^{(b)} = 1.26$ eV in cases a and b, respectively, in Fe. The activation energy for volume self-diffusion calculated from the same model is $Q_B = 2.05$ eV. In Mo they found 2.90, 2.25, and 3.81 eV, respectively. It should be noted, however, that in order to find a value of Q_p for comparison with experiment it is necessary to consider all possible paths of the diffusing atom and to take into account the contribution of each path to the resultant diffusion flux at the given temperature; it is not sufficient to consider only the path which crosses the lowest barriers.

Plishkin *et al.*^{133,134} used a variational procedure to simulate the migration of a vacancy along the core of an edge dislocation with a Burgers vector $\mathbf{b} = (a/2)[110]$ in the fcc copper lattice; they took the splitting of the dislocation into account. The height of the potential barrier to the motion of the vacancy was calculated by a method which began with the relaxation of the microcrystallite with the edge dislocation. The dislocation spontaneously split into two partials, and a stacking fault formed between these partials. The vacancy was formed by removing one of the atoms from the vicinity of the stacking fault or from the core of a dislocation partial.

From this point on the calculation procedure is reminiscent of that in the preceding studies. Analysis of the migration energies for a vacancy in various positions shows that a vacancy can wander rather easily along the plane of a stacking fault in the direction from one dislocation partial to another. The ratio of the diffusion coefficient along this direction to that in the matrix, D_1/D_0 , can be as large as several orders of magnitude. It was concluded in Refs. 133 and 134 that the diffusing species should be transported most intensely along the central part of a stacking fault.

5. GRAIN BOUNDARIES IN POLYCRYSTALLINE MATERIALS

Grain boundaries are the only defects whose atomic structure remains in dispute, although research of the past few years by computer simulation and electron microscopy of bicrystals with a resolution at the level of atomic planes has been of significant help in settling the matter.

The atomic structure of grain boundaries and of grainboundary dislocations (more on this below) determines the mechanisms for grain-boundary slip, the migration of boundaries during recrystallization and plastic deformation, grain-boundary diffusion, and other phenomena in polycrystalline materials. This structure has been the subject of many recent computer calculations. Let us briefly review the methods for describing boundaries.

A plane boundary¹⁰⁾ between grains is determined by

five parameters: Three angles specify the relative rotation of the two grains (two angles specify the direction $\theta / |\theta|$ of the unit vector along the rotation axis in space, where θ is the magnitude of the rotation around this direction), and two angles specify the direction of the unit normal n to the plane of the boundary. These angles are usually specified in a coordinate system tied to the crystallographic axes of one of the grains. Added to the macroscopic parameters θ and n are three microscopic parameters: the components of the vector (r) describing the relative rigid displacement of the grains. The projection of r onto n evidently determines the excess volume of the boundary, i.e., the difference (per unit area of the boundary) between the volumes of the bicrystal and of the corresponding single crystal having the same number of atoms. A boundary for which the rotation axis lies in the plane of the boundary $(\theta \perp n)$ is called a "tilt boundary." At a "twist boundary" we would have $\theta \| \mathbf{n}$. Other boundaries are "mixed."¹³⁵

Let us consider the superposition (1, 2) of two lattices 1 and 2 whose orientations differ by an angle θ and which have at least one common site. If we arbitrarily draw a boundary plane **n** at this superposition, fill the sites of lattice 1 with atoms on one side of this plane, and fill the sites of lattice 2 on the other side, we obtain a bicrystal.

The boundary energy U is defined as the difference between the energy of the bicrystal and that of a single crystal having the same number of atoms, per unit area of the boundary. The atom structure and the boundary depend on θ , **n**, and the particular placement of the boundary plane in the original superposition (1, 2). This placement determines the vector **n**. A minimum of U corresponds to the value $\mathbf{r} = \mathbf{r}_0$. To find \mathbf{r}_0 , the crystals 1 and 2 are initially subjected to a relative displacement as rigid bodies (a rigid relaxation), and this is continued until a minimum value of U is found. A further decrease in the energy is achieved if all the atoms are given the freedom to undergo displacements independently (atomic relaxation). The position of the atoms which corresponds to the minimum of U determines the equilibrium atomic structure of the boundary which is being sought.

Nearly all the calculations of U which have been carried out have used the approximation of a binary atomic interaction.

For arbitrary combinations of θ and **n** it is necessary to find the positions of all the atoms near the surface where grains of macroscopic size come in contact, and this problem exceeds the capabilities of even powerful computers. The problem can be simplifed greatly if there are at least two coincident sites in the (1, 2) superposition. In this case, by virture of translational invariance there will be infinitely many coincident sites in an infinite superposition, and these coincident sites will form a lattice of coincident sites. At certain special values $\theta = \theta_{0,i}$ (*i* = 1, 2, 3,...) the period of the lattice of coincident sites is small, and each Σ th site is a coincident one. If we furthermore choose n in such a manner that the boundary plane coincides with a low-index plane of the lattice of coincident sites then the boundary is a "special" one, its atomic structure is periodic, and it is sufficient to determine this structure for only a single period. Experimentally it turns out that curve of the dependence $U(\theta)$ for a

¹⁰Calculations and observations show that curved boundaries actually consist of butt joints of plane facets.

given low-index direction of the rotation axis has sharp dips at the special angles $\theta_{0,i}$.

Comparatively short periods are found for values $\Sigma \leq 25$. Most of the atomic-structure calculations have been carried out for these special boundaries. In actual polycrystalline materials, these special boundaries constitute no more than 10% of the total number of boundaries; the other boundaries are called "ordinary" boundaries.

A particular case of a special boundary is a twin boundary. Short-period (special) boundaries have a rather regular structure (more on this below). This regularity is disrupted when dislocations from the interior of the grains are captured into the boundary or when θ deviates slightly from a special angle. These deviations are induced by certain specific linear defects: grain-boundary dislocations, of which twin dislocations are an example.

So far, computer calculations have been carried out for only certain special tilt boundaries and twist boundaries in cubic bicrystals. The usual approach is to place a boundary plane running through coincident sites in the central cross section, z = 0, of the rectangular calculation cell. The dimensions of the cell along x and y are the repetition periods of the lattice of coincident sites, l_1 and l_2 ; periodic boundary conditions are imposed at the boundaries of the cell. The dimension of the cell along the z axis, l_3 , is also of the order of the period of the lattice of coincident sites. In the initial position, all the atoms are fixed at the corresponding sites of the (1, 2) superposition, and the energy of the structure, U^{0} , is calculated. A rigid relaxation is then carried out. One half of the bicrystal (z > 0) is displaced as a rigid body with respect to the other half $(z \le 0)$ by a distance $r = r_1$ at which the energy of the system reaches a minimum (U^{1}) . For this purpose, r_x and r_y are varied within the limits of l_1 and l_2 (the coincident sites undergo transitions from the boundary into the interior of the crystals, as is easily verified by performing a relative displacement of lattices 1 and 2 drawn on tracing paper. The dimension r_z does not exceed a few tenths of the distance between atoms (otherwise, a gap would form at the boundary plane, and U would increase dramatically). The positions of the atoms at and near the boundaries $\pm (1/2)l_3$ of the calculation cell are then fixed, and the other atoms are allowed to relax until an absolute minimum energy U^2 is reached. The sequence of steps in finding U^2 is slightly different in case of ordinary boundaries.¹³⁶

Since it has not been shown that the minimum found is in fact the absolute minimum, we need to verify whether the minimum U^1 found in the stage of the rigid relaxation is unique and, if it is not, we need to arrange an atomic relaxation of the configurations corresponding to the other minima U^1 and select the smallest from the set of resulting values $U_2^{(1)}, U_2^{(2)}, U_2^{(3)}, \ldots$ Structures corresponding to other minima may be regarded as grain-boundary stacking faults.

The results provided by computer simulation of boundaries up to 1978 are covered in Chapter V of Ref. 135. These results confirmed the existence of dips on the $U(\theta)$ curves and revealed similar structural elements at boundaries with different values of θ . Calculations¹³⁷ carried out for fcc crystals and an analysis¹³⁸ of the earlier work have shown that these structural elements are combinations of Voronoĭ polyhedra



FIG. 26. Structure of a [100], $\Sigma = 5$, tilt boundary in aluminum (top) and density of the vibrational levels of various atoms in it.¹⁴⁸

which include groups of close-packed (tetrahedra, octahedra, and trigonal prisms) separated by more-porous interlayers, but without interstitials capable of accepting an extra atom (compact polyhedra¹³⁹). Figure 26 shows as an example a symmetric [100], $\Sigma = 5$, tilt boundary in Al, where pentagonal bipyramids are triagonal prisms with caps have been singled out. The results of systematic calculations for 50 different special [100], [110], and [111] tilt boundaries in fcc crystals are reported in Ref. 140; the excess volume of the boundary and the order in which the polyhedra are arranged are also given there. In general, compact polyhedra form already during the stage of rigid relaxation (so that there are no coincident sites at the boundary), not during atomic relaxation.

Trihedral prisms with caps and pentagonal bipyramids are observed at [100] and [110] tilt boundaries in a bcc lattice, according to calculations with various potentials.¹³⁹ The structure of the bcc lattice is more porous than that of an fcc lattice. If it is to be stable with a central potential, the interactions in to coordination spheres must be taken into account; together, these two spheres contain 14 "nearest" neighbors. Consequently, although tilt boundaries in bcc metals also consist of compact polyhedra the packing of atoms in them is not as close as in fcc metals, and the atomicrelaxation stage is just as important as the rigid displacements in finding the positions of the atoms.¹⁴¹ The structure of the boundary is thus more symmetric, and coincident sites are found in it more frequently than in fcc crystals.

Nichols¹⁴² has carried out structural calculations on tilt boundaries with angles lying between two special angles; he found that as θ is varied there is a progressive change in the surface concentration of the polyhedra of the various types.



FIG. 27. Symmetric [0001], $\Sigma = 7$, tilt boundary in α -titanium¹⁴⁵ (hcp). Circles and crosses—Atoms in adjacent (0001) planes; hatched region around atom A—a 10× enlargement of the vibration amplitude of this atom at 300 K; at the right—combinations of octahedra and tetrahedra in a defect-free hcp lattice (see the text proper).

Structural calculations on twisting boundaries^{143,144} have revealed no fundamental differences from tilt boundaries.

In what is so far the only study of hcp crystals,¹⁴⁵ Hashimoto *et al.* studied the structure and vibration spectrum of the atoms (more on this below) at a [0001], $\Sigma = 7$ (1320), tilt boundary in α -Ti with the help of a Lennard-Jones 6–12 potential. Figure 27 shows the relaxed structure of the boundary. The repetition period contains two deformed triangular prisms with two semioctahedral lateral caps (ABCD'EC'FB) and four deformed tetrahedra (AD'F'C) and ACED. On the curves of the state density $g(\omega)$ of the type in Fig. 26 the atoms A and D have low-frequency resonant modes.

The above calculations dealt with the structure of the boundaries at a temperature of 0 K. In an effort to calculate the frequencies of the thermal vibrations, which determine the vibrational entropy of a boundary, Provan and Bamiro146 used the Einstein model which has each atom vibrating independently with a frequency ω_E in the potential well formed by the neighboring atoms, which are assumed fixed. The frequency ω_E is determined by the particular interatomic potential which is used. There are some more rigorous methods for calculating the local density of vibrational states of each atom in the calculation cell: 1) diagonalizing the dynamic matrix for all the atoms of the calculation cell; 2) analyzing the vibrations by molecular dynamics; and 3) the recursive method of Ref. 147, which involves calculating the coefficients and writing a Green's function as an infinite fraction. The last of these methods is the one which requires the least computer time. It was used by Hashimoto et al.¹⁴⁸ to calculate the vibrational spectra of the atoms [the local state density $g(\omega)$] of [001], $\Sigma = 5$ and $\Sigma = 11$, tilt boundaries (two distinct configurations with slightly different energies U), in aluminum with the help of a Morse potential. The results for the $\Sigma = 5$ boundary, with the lower energy, are shown in Fig. 26. The atoms E, which is at a vertex of a pentagonal bipyramid and which lies farther than the other atoms from the neighbors, has a low resonant frequency. The calculations show that this circumstance causes a pronounced increase in the entropy S and a significant decrease in the free energy of the configuration F = U - TS.

Dynamic simulation of thermal vibrations can be used to study the way in which the structure of a bondary forms as a melt solidifies.¹⁴⁹ So far, calculations have been carried out for only a two-dimensional model because of limited computer time. Let us outline this method. The positions of the atoms in grains 1 and 2, whose orientations differ by a given angle θ , are specified at the opposite straight edges of the working cell. The gap between the grains is filled with a liquid, i.e., with atoms whose average kinetic energy exceeds $kT_{\rm m}$. The "pressure" is adjusted by specifying the width of this gap. The temperature (T) and the pressure (p) of the liquid are lowered in accordance with a specified program, and the liquid solidifies; the relaxation of the grain-boundary interlayer does not occur at 0 K, as it does in the static calculations. Cotterhill et al. 149 carried out calculations for a part of a symmetric $\Sigma = 21$ [111] boundary containing 400 atoms, using 6000 time steps Δt (6000 $\Delta t = 10^{-10}$ s). The structure of the resulting boundary depends on not only the instantaneous values of T and p but also on the way in which T and p have been changing. After $\sim 50\Delta t$, however, they reach equilibrium values. Increasing T results in increases in the width and porosity of the boundary; increasing p at a nonzero T leads to a more compact structure. Although the boundaries of gains 1 and 2 are always specified by straight lines, the final boundary is not straight in all the cases [T(t)], p(t)] studied. This circumstance implies that this boundary is quite mobile both at the time of solidification and after, if it is held at an elevated temperature. On the other hand, clearly defined mirofacets are also absent.

Computer simulation can also be used to study the structure of interphase boundaries. For example, an important topic in the crystallography of phase transitions in steel is the structure of the interface between fcc (γ) and bcc (α) lattices. One wishes to determine the conditions under which the Kurdyumov-Zachs, $\{110\}_{\alpha} \parallel \{111\}_{\gamma}, \langle 1\overline{1}1 \rangle_{\alpha} \times \langle 1\overline{1}1 \rangle_{\gamma}$ Nishiyama-Wasserman, and $\{110\}_{\alpha} \| \{111\}_{\gamma}$ $\langle 001 \rangle_{\alpha} \times \langle 01\overline{1} \rangle_{\nu}$, orientational relations apply. Complete accomodation of the lattices at a phase boundary can be achieved by introducing one or several families of mismatch dislocations and parallel projections one or more atoms high at the interface. The only calculated results available so far are the parameters of these families of line defects, as functions of the ratio of lattice constants a_{α} and a_{γ} and of the angle (ψ) through which the α lattice is rotated with respect to the γ lattice around the $[111]_{\gamma}$ direction. While $\psi = 0$ is assumed for the Nishiyama-Wasserman relations, we have $\psi = \pm 5.26^{\circ}$ for the Kurdyumov-Zachs relations.¹⁵⁰ No atomic-structure calculations have been reported for the cores of mismatch dislocations and projections or for boundaries for arbitrary values of ψ and **n**. Results of this type should reveal whether the boundary model of Ref. 150 actually corresponds to a minimum of the free energy.

6. STRUCTURAL DEFECTS IN AMORPHOUS METALS

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Amorphous metals are a new field of application of computer simulation. They are studied by constructing

model structures of randomly positioned close-packed spheres.¹⁵¹ The size of the calculation cell and periodic boundary conditions are specified, and the positions of the centers of the hard spheres of a given radius are found with the help of a random-number generator. The filling of the calculation cell is continued until there are no longer any places to add spheres without overlapping adjacent spheres. The interatomic potential $\varphi_{ij}(r)$ is then specified, and a relaxation is carried out; i.e., those displacements of the atoms which correspond to a minimum of the energy (E) of the system at the given volume V are found. The pressure exerted on the boundary atoms, p, is calculated, and the volume V is varied by displacing the boundary atoms until the energy E reaches a minimum at $V = V_0$ and p = 0.

Extracting information on the macroscopic properties of these structures requires a statistical analysis. Until recently, the only method which was used was to find the radial distribution function of interatomic distances and to compare it with experimental data. The data file containing the coordinates of all the atoms in the calculation cell obviously contains far more information. A method which has been proposed^{152,153} for describing this information deals with the local stress tensor (atomic-level stresses) at the position of atom *i*:

$$\sigma^{\alpha\beta}(i) = \frac{1}{2\Omega_0} \sum_{j \neq i} \frac{\mathrm{d}\varphi(r_{ij})}{\mathrm{d}r_{ij}} \frac{r_{ij}^{\alpha}r_{ij}^{\beta}}{r_{ij}}; \qquad (34)$$

where r_{ij} is the distance between atom *i* and its neighbor *j*, and Ω_0 is the volume of the Wigner-Seitz polyhedron around the atom *i*. A second structural characteristic consists of the symmetry coefficients of the surroundings of atom *i*: the coefficients $\varepsilon_n^{l,m}(i)$ in the expansion in spherical harmonics $Y_i^m(\theta_i,\varphi_i)$ of the expression for the change (ΔE_i) in the energy of atom *i* when it is displaced by $\Delta \mathbf{r}_i$, while the neighboring atoms are held fixed:

$$\Delta E(i) = \sum_{n=1}^{\infty} \frac{\partial^n E}{\partial \mathbf{r}_i^n} \frac{|\Delta r_i|^n}{n!}.$$
(35)

In the equilibrium state we would have

$$\frac{\partial^{n} E}{\partial \mathbf{r}_{i}^{n}}\Big|_{eq} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \varepsilon_{n}^{l, m}(i) Y_{l}^{m}(\theta_{i}, \varphi_{i}).$$

Of primary interest are the invariants $\alpha_0 = \varepsilon_2^{0,0}$ (which represent a bulk modulus) and

$$\beta = \frac{1}{\alpha_0} \sqrt{\sum_{m=-2}^{2} |\varepsilon_2^{2, m}|^2}, \qquad (36)$$

which is a measure of the deviation of the surroundings of the atom from spherical symmetry. Calculations were carried out in Ref. 153 with the potential φ_{ij} for iron. The values of α_0 and β were calculated for each atom, and the invariants of the tensor $\sigma^{\alpha\beta}$, in particular, the pressure $p = \frac{1}{3} \sum_{\alpha} \sigma^{\alpha\alpha}$ and the Mises invariant

$$\begin{aligned} \tau &= \left\{ \frac{1}{3} \left[\frac{1}{2} (\sigma_1 - \sigma_2)^2 + \frac{1}{2} (\sigma_2 - \sigma_3)^2 + \dots \right. \right. \\ &+ \frac{1}{2} (\sigma_3 - \sigma_1)^2 \right] \right\}^{1/2}, \end{aligned}$$

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FIG. 28. Three adjacent layers (a, b, c), 0.37 nm thick with an overlap of 0.057 nm, oriented parallel to the plane of the displacement in the calculation cell of amorphous iron. Squares—Central atoms of n-type defects; triangles—of p-type defects; solid curves—surrounding large n-type defects; dashed curves—surrounding large p-type defects.¹⁵³

were also calculated. All the atoms were classified into 4kgroups on the basis of the numerical values of each of the kinvariants. The groups with the smallest and largest values each contain 21% of the total number of atoms. There are correlations between the values of the various invariants for a given atom. It turns out that the atoms of the extreme groups combine into clusters of 10-20 atoms, which may be regarded as defects of the amophous structure. Defects with a low density ρ (~10% lower than the average density $\bar{\rho}$; these are regions of dilatation, called "n-type defects") are analogs of vacancies in crystals but are spread out to a greater extent. Defects with densities 10% higher than $\bar{\rho}$ (compression regions; "p-type defects") are analogs of interstitial atoms. The numbers of n-type and p-type defects are nearly identical. The two types frequently occur in pairs (Fig. 28). There can be a mutual annihilation of n-type and ptype defects, in the manner of Frenkel' pairs. Simulation of the annealing of an amorphous metal has made it possible to reproduce those changes in the radial distribution function of the atoms which are associated with annihilation and which have been observed experimentally.154

Atoms in defects having extreme values of τ have large values of β . In these regions, an applied tangential stress nucleates plastic displacements. The dynamics of the formation of these displacements has been studied¹⁵⁵ in a calculation cell of 2067 atoms with periodic conditions at the boundaries, where the shear deformation γ was specified. This deformation was increased in steps $\Delta \gamma = 0.1-0.2\%$; in each step, an atomic relaxation was carried out, and the atomic displacements $\Delta u_{\alpha}(i)$, the strain $\Delta \varepsilon^{\alpha\beta}(i)$, and the energy changes



FIG. 29. Displacements of atoms during shear deformation.¹⁵⁵ The wide arrows show the average displacements.

$$\Delta E (i) = \sum_{\alpha,\beta} \sigma^{\alpha\beta} \Delta \varepsilon^{\alpha\beta} + \sum_{\alpha,\beta,\gamma,\xi} C^{\alpha\beta\gamma\xi} \Delta \varepsilon^{\alpha\beta} \Delta \varepsilon^{\gamma\xi}$$

were calculated. The local elastic constants $C^{\alpha\beta\gamma\zeta}$ were calculated as in (34). Curves of ΔE as a function of γ have breaks accompanied by average displacements of the atoms in the τ defects by distances of the order of the interatomic distance. These displacements are directed in such a manner that the elastic shear energy relaxes (Fig. 29). An irreversible deformation is localized in regions $\sim 4a$ in size. There are correlations among Δu , p, the shear stresses σ_{xy} , the elastic moduli $C^{\beta\gamma\zeta}$, and the distribution of Voronoĭ polyhedra.¹⁵⁶

In the simulation of self-diffusion in an amorphous metal,¹⁵⁷ an atom is removed from the metal, and the heights of the potential barriers opposing hops of each of the surrounding atoms to the new vacancy are determined. There is a considerable spread in the heights of these barriers.

The results discussed above show that the concept of a localized structural defect can be applied to amorphous objects as well as to crystals. We can therefore speak in terms of defects in solids in general.

7. OUTLOOK FOR FURTHER USE OF COMPUTER SIMULATION TO STUDY DEFECT STRUCTURES

Important new results can be expected in the upcoming decade in three basic directions.

1. Simulation of defect structures in systems consisting of atoms of several species (solid solutions with concentration inhomogeneities and ordering and decay processes taken into account; intermetallic compounds; amorphous metals and alloys) and simulation of reactions between, and changes in the structure of, various defects in such systems.

2. Simulation of the behavior of defect structures in solids subjected to combinations of effects: stresses, heating

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and cooling, bombardment with fast particles, electric and magnetic fields, etc.

3. Simulation of the defect structures at the surfaces of solids and at internal interfaces (grain boundaries in polycrystalline solids, interphase boundaries, and epitaxial films) and simulation of the changes in the structure of surface defects, in particular, adsorption and catalysis (topics which we have not discussed here).¹¹⁾

What developments can we expect in methods for computer simulation? As can be seen from the examples discussed here, the process of using a computer to simulate the structures and structural changes of defects is becoming progressively more distinct from the process of solving a system of equations of motion for atoms treated as spheres connected by springs (interatomic forces) which will break if stretched too far. The reason for this trend lies in the complicated nature of the interatomic interactions in solids. The results obtained from simulations agree with experimental results only if the actual nature of the crystal (or amorphous object)-a complicated quantum-mechanical system of atomic cores and electrons-is taken into account in a comprehensive way. A rigorous complete solution of the quantum-mechanical problems in the determination of the structures of even simple defects, on the other hand, is still a long way off in the future because of the limited capabilities of computers (and it may also be necessary to develop some new approaches). We should therefore expect a further development of approximate methods for describing the interatomic interactions, with an accuracy significantly better than that of existing methods.

Despite the complications in calculations under these circumstances, there is hope that results of theoretical and experimental research on the structures of defects and progress in computational capabilities will make it possible, at some time not too far in the future, to use a computer to "run through" the effects of stresses, temperature fields, etc., on given defect structures in solids and to use this approach to find ways to produce new materials with desirable combinations of properties.

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¹¹We have considered only metals and alloys in this review. We might also expect that further work will be carried out in the three directions enumerated above to simulate defects in nonmetallic crystals and amorphous objects, including biopolymers.

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