Stable Atomic Configurations for an Interstitial in Copper*

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The stability of various atomic configurations for an interstitial is investigated in a model representing copper. For the interaction between the lattice ions, a Born-Mayer and a Morse potential are used. Two equilibrium configurations are found for an interstitial. For the two stable positions the formation energies and the changes in volume of the crystal arising from the interstitial are calculated. The calculations show that the crowdion and the "body-centered" interstitial are unstable.

THE different stable atomic configurations, formation energies, and changes in volume of the crystal for an interstitial in copper are calculated with the help of the electronic digital computer Z22[1] using a general method developed by Tewordt.[2] In this method the lattice distortion around the interstitial is determined by an iteration process minimizing the energy. During the relaxation of the lattice the interstitial migrates from an arbitrarily chosen position into an equilibrium configuration. In all calculations a sufficient number of atoms around the mobile interstitial is treated as movable discrete particles. For the interaction between a pair of ions at separation r the Born-Mayer potential,

$$V_1(r)=0.053\exp[13.9(r_0-r)/r_0]\text{ ev},$$
$$(r_0=a/\sqrt{2},\ a \text{ is the lattice constant})$$

given by Huntington,[3] and the Morse potential,

$$V_M(r)=0.343\{\exp[7.78(R_0-r)/R_0]$$
$$-2\exp[3.89(R_0-r)/R_0]\}\text{ ev},\quad (R_0=0.794a),$$

given by Girifalco-Weizer,[4] are employed. The electronic contributions to the relaxation of the lattice due to the redistribution of the electrons are neglected.

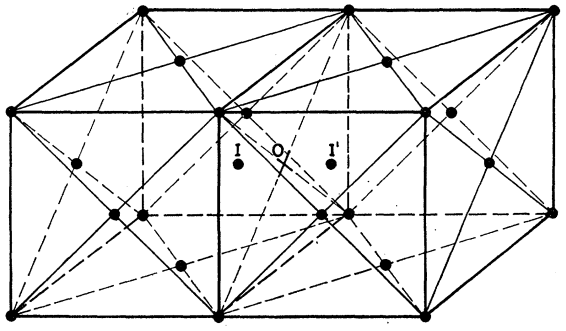

FIG. 1. The stable atomic configuration "A" for an interstitial in a cubic face-centered lattice. Two elementary cubes of the lattice are drawn. I is the interstitial and I' the atom which lies relative to one of the cube faces symmetrically to the interstitial. O is the regular site of the atom I'. The distance between I and I' is $0.6a$.

The stability of various interstitial configurations is investigated. The most important new result is that two equilibrium configurations are found for an interstitial. The calculations performed with the potentials V_1 and V_M show that the configuration "A", first considered by Huntington and Seitz,[5] is stable. Recently Gibson *et al.*[6] and Johnson *et al.*[7] found the same result with the potential V_1 in models very similar to that used here. In the stable "split" configuration "A", shown in Fig. 1, the interstitial and one next-neighbor atom are symmetrically located relative to one of the elementary cube faces along a cubic axis passing through the cube center. The stability of configuration "B", which is considered for the first time, is found using the potentials V_1 and V_M. In the stable "split" configuration "B", which is shown in Fig. 2, the interstitial and one next-neighbor atom are symmetrically located relative to a cube corner along a [111] axis. If the interstitial is displaced slightly from its position in configuration "B" toward surround-

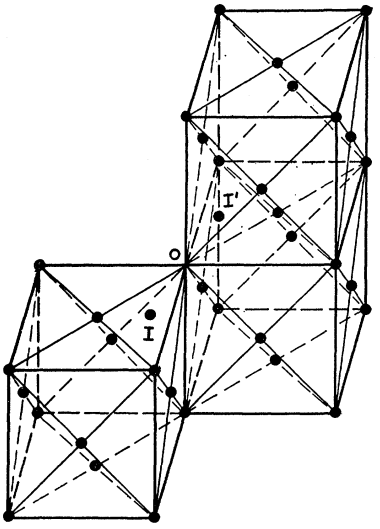

FIG. 2. The stable atomic configuration "B" for an interstitial in a cubic face-centered lattice. Three elementary cubes of the lattice are drawn. The interstitial I and the atom I' are symmetrically located relative to the cube corner O along a [111] axis. O is the regular lattice site of the atom I'. The distance between I and I' is $0.6a$.

* Partially supported by U. S. Atomic Energy Commission.
[1] Electronic digital computer Zuse 22, Institut für Angewandte Physik, Universität Münster, West Germany.
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[7] R. A. Johnson, G. H. Goedecke, E. Brown, and H. B. Huntington, Bull. Am. Phys. Soc. **5**, 181 (1960).

ing crowdion, "body-centered," or "A" interstitial positions the calculations show that the interstitial returns to its position in configuration "B". Configuration "B" is separated from possible surrounding interstitial configurations by energy barriers of about 0.3 ev.

The interstitial configuration with the interstitial in the "body-centered" position is found to be unstable. Calculations performed with V_1 and V_M show that the interstitial moves from the elementary cube center along a cubic axis about $0.2a$ into the equilibrium configuration "A". The migration energy for an interstitial moving between adjacent "A" configurations turns out to be 0.1 ev. Furthermore, the crowdion is found to be unstable. Using V_1 or V_M the extra atom of the crowdion configuration moves into a next neighbor position which is equivalent to the interstitial position in configuration "A." These results agree with those found with the potential V_1 by Gibson *et al.*[6]

The number of atoms around the interstitial treated as movable discrete particles is about 150 for the interstitial configuration "A" and about 50 for the interstitial configuration "B". Using potential V_1, the change in volume of the crystal arising from the interstitial is found to be 1.126 atomic volumes for configuration "A" and 1.432 atomic volumes for configuration "B". The contributions to the formation energy of an interstitial arising from the potential V_1 turn out to be 3.548 ev for configuration "A" and 4.098 ev for configuration "B".

A more detailed description of the calculations is given in a paper which will be published in the *Zeitschrift für Physik*.

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Theory of Many-Particle Systems. II. Superconductivity*

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A fermion system with a simple attractive interaction is discussed with the aid of time-dependent correlation functions. Although perturbation theory is inapplicable, a sequence of correlation approximations described in the first paper of this series can be employed. The lowest approximation in the sequence expresses the two-particle correlation function in terms of single-particle functions and leads to the Hartree approximation; the second expresses three-particle correlation function in terms of one- and two-particle correlation functions and leads to the time-dependent correlation functions that characterize the superconducting model of Bardeen, Cooper, and Schrieffer. In the second section of this paper these correlation functions are determined and the thermodynamic properties of the superconductor are calculated from them.

In the third section of the paper, the electromagnetic effects of the superconductor predicted by the Bardeen-Cooper-Schrieffer time-dependent correlation functions are considered. Their unsatisfactory description of current conservation is indicated and overcome in the fourth section by a more accurate solution valid at nonvanishing temperature. This solution predicts different diffusive properties but the same Meissner effect and superconductive behavior, since the longitudinal current correlation function is modified while the transverse current correlation function is not.

The fifth section of the paper is devoted to the properties of a pure superconductor which depend on the lifetimes of the single-particle excitations. The effect of these lifetimes on the static electrical conductivity is determined, and it is shown that they do not destroy supercurrents although they eliminate a gap in the single-particle excitation spectrum. Their effect on the thermal conductivity is also calculated using heat current correlation functions. It is shown that a model which treats the lifetime of the single-particle excitation due to lattice interactions as constant yields results in agreement with observed thermal conductivities.

1. INTRODUCTION

IN a previous paper,[1] a formalism for discussing systems with many particles was developed, and certain systematic approximation techniques were outlined. A sequence of correlative approximations which did not involve expansion in powers of the potential was proposed and shown to yield many of the features which characterize these many-particle systems. Before extending this general formulation, it seems desirable to illustrate the techniques introduced by applying them to a specific problem. Probably the most illuminating example on which to employ them is a simplified model of superconductivity. On the one hand, this example provides a rather stringent test of any approximation scheme, since the model is known to have features which cannot be derived by expansion in the coupling constant. On the other hand, the application of a

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[1] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959), hereafter referred to as I.