Huang scattering and extinction length of conduction electrons

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Calculations are presented for conduction-electron scattering on dislocation loops in Al. The detailed agreement with the experiment demonstrates that scattering on extended lattice distortions must be treated with a dynamical scattering theory. An extinction length for conduction electrons is introduced, such that lattice distortions varying gradually on the scale of the extinction length can largely be followed adiabatically by the electron and cause little scattering. The extinction length in Al is 25 Å.

I. INTRODUCTION

In calculating the scattering of electrons on extended lattice defects such as dislocations or stacking faults, one is faced with the problem of a scattering process that is neither weak nor localized. It is not immediately clear how the variations of the electron wave function in the extended region of the defect reflect the continuous changes in the lattice spacing and at the same time the discontinuity at the lattice imperfection. I propose to introduce, in analogy with dynamical scattering of x rays, an extinction length for conduction electrons as an important material constant with which the scale of lattice distortions should be compared.

Because the predominantly small angle scattering caused by such defects can be detected only with special methods, experimental studies are also very difficult. Recent measurements using surface-Landau-level resonance (SLLR) in Al (Ref. 1) have shown that the scattering on lattice defects is very anisotropic and that for electron states with wave vectors near Brillouin-zone boundaries, the near-Bragg-reflection scattering plays a dominant role. In the present paper I wish to discuss the SLLR results[1,2] by describing the scattering of electrons on dislocation loops in terms of Huang scattering in which the scattered-wave amplitudes from all displaced ions are summed within the first Born approximation. Following that, a comparison of calculational results with the experiment shows that such a kinematical theory can be successfully applied, but only to relatively small dislocation loops. The description of larger defects requires a treatment similar to the dynamical theory of x-ray scattering. In particular, an extinction length can be defined, which is a measure of the spatial extent of lattice distortions beyond which the kinematical theory is no longer applicable. For the electrons studied by SLLR in Al (Ref. 1), the extinction length is determined both by experiment and theoretical estimate to be of the order of five lattice constants.

II. HUANG SCATTERING

The main features of the exact theory of Huang scattering as applied to x rays or neutrons[3] can be demonstrated with a simple model of a cluster of vacancies or interstitials surrounded by a spherically symmetrical elastic displacement field. The cluster consists of n_c defects, enclosed within a sphere of radius R_c, outside of which the radial displacements of the ions from their ideal lattice positions $\vec{R}_n$ are given by $\vec{t}_n = (\vec{R}_n/R_n^3) n_c \Delta V / 4\pi$, where ΔV is the lattice relaxation volume per defect. Experimentally determined values of the relaxation volume in Al are $(-0.05 \pm 0.05)V$ for an isolated vacancy, and $(+1.9 \pm 0.2)V$ for an isolated interstitial, where V is the atomic volume.[4] It has been shown that these defects in Al agglomerate into dislocation loops.[5] For example, a vacancy dislocation loop develops from the agglomeration of vacancies into a platelet within one atomic plane, causing the neighboring atomic planes to relax inward to fill in the empty volume. For large loops $\Delta V \cong -V$ (vacancies) or $\Delta V \cong +V$ (interstitials). For such a cluster, the scattering-amplitude structure factor is given to a good approximation for small q by

$$F(\vec{q}+\vec{h}) = n_c j_0(qR_c) \times [(\mp 1 - \Delta V/V) - (\Delta V/V)\vec{q}\cdot\vec{h}\, q^{-2} - (|\Delta V|/V)\tfrac{1}{3} h R_c], \quad (1)$$

where $\vec{h}$ is any reciprocal-lattice vector (including $h=0$), $q \leq h/2$ for $h \neq 0$, j_0 is the zeroth spherical Bessel function, and R_c is the loop radius. The first two terms in (1) correspond to, in the terminology of x-ray scattering,[3] the small-angle and Huang terms, respectively. The small-angle term describes the change in ion density resulting from the vacancies (−1) or interstitials (+1) and the corresponding far-field

dilatation ($\Delta V<0$) or compression ($\Delta V>0$) of the lattice. The Huang term reflects variations in $\vec{h}$ due to far-field radial displacements; the large displacements within the sphere are included in the third term in (1). An electron entering from the perfect lattice into the distorted region will scatter on a nearly periodic defect potential $W(\vec{r})$ of the displaced ions which will be most effective near a Bragg peak ($q\to 0, h\neq 0$).

To describe the scattering of electrons in Al within the first Born approximation one can determine the matrix elements $M_{kk'}=\langle\psi_k|W(\vec{r})|\psi_{k'}\rangle$ using 4-orthogonalized plane-wave (OPW) wave functions $\psi_{\vec{k}}=\sum a_j\exp[i(\vec{k}+\vec{g}_j)\vec{r}]$, where $\vec{g}_j$ are reciprocal-lattice vectors. Generally,

$$M_{kk'}=\sum_{ij} a_i^* a_j W(|\vec{q}+\vec{h}_{ij}|)F(\vec{q}+\vec{h}_{ij}), \tag{2}$$

where $\vec{q}+\vec{h}_{ij}=\vec{k}'-\vec{k}+\vec{g}_j-\vec{g}_i$, and $W(|\vec{q}+\vec{h}|)$ is the Al pseudopotential form factor. Despite the singularity of F at $q\to 0, h\neq 0$, $M_{kk'}$ is finite for all q's. The rate of scattering Γ_k from state $\vec{k}$ into all final states on the Fermi surface caused by N defects agglomerated into clusters of n_c each, is given by

$$\Gamma_k=(1+\lambda_k)^{-1}(N/n_c)\sum_{k'} 2\pi\hbar^{-1}|M_{kk'}|^2\delta(\epsilon_k-\epsilon_{k'}), \tag{3}$$

where λ_k is the electron-phonon mass enhancement factor.[6] A result of numerical calculations according to (2), (3), and a more exact version of (1) valid for all q, using 4 OPW wave functions of Pfändner *et al.*,[7] is shown in Fig. 1(a) for the case of vacancy agglomeration. The interdependence of n_c, R_c, and $\Delta V/V$ was based on simple geometrical considerations, assuming that for n_c between 4 and 7 a platelet configuration starts to develop and gives rise to lattice relaxation. The minimum in Γ for R_c approximately equal to the lattice constant results from a partial cancellation of the small-angle and Huang terms in expression (1). With the progressing decrease of $\Delta V/V$ towards the value -1 for larger loops, the small-angle scattering disappears as near-normal ion density is reestablished within the cluster. At the same time the Huang term becomes more important for those states ψ_k which have a clear multi-OPW character, such as c and d [Fig. 1(d)]. In comparison, electrons in state A which cannot be scattered through a vector close to $\vec{g}_i$ react weakly to the lattice distortion. The Huang scattering is therefore very anisotropic.[8]

Figure 1(c) shows experimental results on a quenched sample (for details see Ref. 1). A comparison[1,2] of these results with SLLR annealing curves for defects introduced by irradiation has led to the identification of vacancy agglomeration as the cause of the observations, and to an estimate of the vacancy concentration lying between 2 and 5 ppm. Electron-microscope observations[5] of vacancy loops have shown that with increasing annealing temperature T the radius R_c continues to grow up to 400 K and reaches $R_c>100$ Å well below 300 K. Therefore the shape of the curves in Fig. 1 can be compared assuming that R_c increases monotonically with T. The agreement is good, since the most striking features, i.e.,

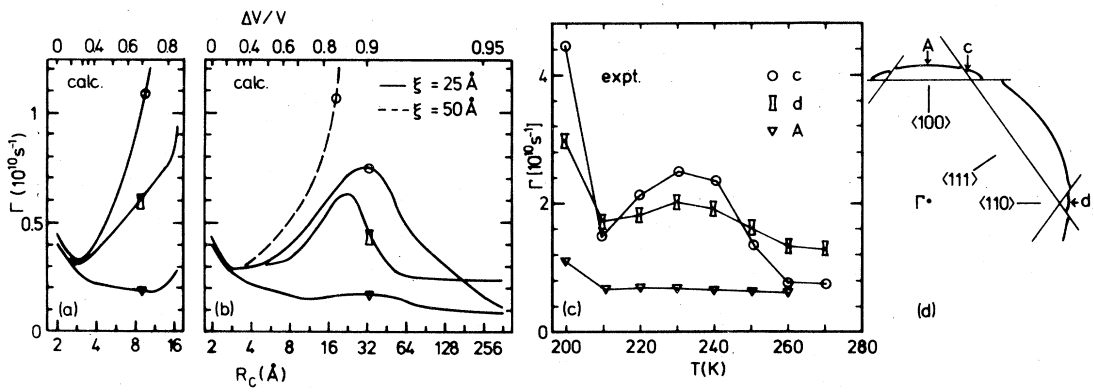

FIG. 1. Calculated and experimentally determined scattering rates Γ for three points on the Fermi surface of Al versus vacancy-dislocation-loop radius R_c. (a) Kinematical theory [Eq. (1)] correctly predicts the scattering minimum and anisotropy resulting from the long-range radial dilatation of the lattice (Huang scattering) characterized by a relaxation volume $\Delta V/V$. A vacancy concentration of 1 ppm was assumed. (b) Corrections for dynamical scattering effects [Eq. (4)] become important for larger loops for which R_c is comparable to the extinction length ξ. (c) The growth of the vacancy clusters into dislocation loops was followed with SLLR (Ref. 1) in an isochronal annealing program for a quenched sample. An independent estimate of the vacancy concentration is between 2 and 5 ppm. (d) The locations of the three points are shown on the central (110) slice of the Al Fermi surface.

the minimum in Γ_c and Γ_d for low R_c and the scattering anisotropy between points A, c, and d, are correctly reproduced by the theory. The absolute values of the scattering rates compare very well, e.g., Γ_A on medium-size loops ($R_c = 8$ Å) is calculated (without adjustable parameters) to lie between 0.4 and 1.0×10^{10} s^{-1} for the estimated 2 to 5 ppm vacancy concentration, while the measured value is 0.7×10^{10} s^{-1}.

SLLR measurements on irradiated Al (Refs. 1 and 2) showed strong anisotropy also for scattering on dislocation loops of interstitials, the anisotropy of related points on the Fermi surface being inverted compared to the case of dislocation loops of vacancies (Ref. 1, Fig. 3). This defect asymmetry follows from the change of sign of ΔV in the Huang term in (1) and has also been reproduced by the numerical calculation, e.g., $\Gamma_c/\Gamma_d > 1$ for vacancy loops, $\Gamma_c/\Gamma_d < 1$ for interstitial loops. The conclusion is that the structure factor $F(\vec{q}+\vec{h})$ describes the scattering for conduction electrons as well as for x rays or neutrons. There is, however, a quantitative difference which will be discussed in the following.

III. EXTINCTION LENGTH

In Fig. 1(c), the scattering rates Γ_c and Γ_d, which at first increase due to Huang scattering, reach a maximum around 240 K and then decrease with progressing agglomeration. This decreasing behavior is also very anisotropic since it is not observed for Γ_A (see also Ref. 1, Fig. 1). Thus the kinematical theory, i.e., the first Born approximation, which correctly predicts the increase due to Huang scattering, gradually loses its validity for large loops [compare Figs. 1(a) and 1(c)]. The reason for this is that the kinematical treatment fails to take into account the modification (due to scattering) of the incident wave within the distorted region of the lattice. This is a situation analogous to the diffraction of x rays or neutrons by single-crystal samples thicker than the extinction length ξ.

For a dynamical treatment of the scattering of conduction electrons on extended lattice defects the distorted region of the lattice should be regarded as a diffracting medium with a Fermi surface and electron wave functions slightly changed compared to the surrounding perfect lattice. As the simplest case, one may consider the propagation of two Bloch waves—the primary and the diffracted—through such a medium. In the undistorted lattice, the incident electron is represented by the primary wave only. As the electron penetrates the distorted region, scattering causes the amplitude of the diffracted wave to increase and that of the primary wave to decrease. This cannot continue indefinitely since the reverse scattering process soon becomes equally important. As in dynamical scattering theories (e.g., for fast electrons used in transmission electron microscopy[9]) it can be shown that the dynamical equilibrium between the two wave amplitudes forces a modulation of the amplitudes with a wavelength equal to the extinction length ξ. A fraction of the incident intensity is transferred back and forth between the primary and diffracted waves in a fashion similar to coupled pendulums. The wavelength of this beat pattern is $\xi = 2\pi/\Delta k$, where Δk is the difference between the wave vectors of the primary and diffracted waves. Both of these waves are independent electron wave functions in the perfect lattice, they behave as coupled in the diffracting medium only because they are driven by the incident wave which is not a wave function of this medium. This coupled mode is a result of the coherent scattering on all the ions of the distorted lattice, the same scattering that has been included in the scattering structure factor in (1). Therefore, since the coupled mode gives rise to a coherent transmitted wave even over lengths much larger than ξ, the scattering on mild lattice distortions that are very gradual on the scale of ξ has been overestimated by the calculation based on (1). The kinematical theory of (1) remains valid in the limiting case of a scattering medium with dimensions smaller than ξ. Therefore it is the lattice distortions that vary rapidly on the scale of ξ that primarily give rise to the scattered waves and to the reduced amplitude of the transmitted wave.

The two-wave model just discussed is only a rough approximation for conduction electrons in Al for which a large number of diffracted waves are excited simultaneously. Nevertheless, the most important effects of the dynamical scattering can be demonstrated by introducing a single averaged extinction length $\bar{\xi}$ for all electron states on the Fermi surface. As an estimate, $\bar{\xi} = 2\pi/\Delta k_g$, where Δk_g can be taken to be the average gap at the (200) Brillouin-zone boundary between the second and third zone sheets of the Fermi surface. Then $\bar{\xi} = 24$ Å. Since $\Delta k/k_F \approx W(g_i)/\epsilon_F$, where k_F and ϵ_F are the Fermi wave vector and energy, respectively, the extinction length for conduction electrons is much shorter than for fast electrons (10^3 Å), x rays (10^4 Å), or neutrons (10^5 Å). Note that the extinction length is a measure of the strength of the lattice potential and is not directly related to the mean free path between scattering events, which for the SLLR samples is of the order of 10^{-2} cm.

One can attempt to correct the calculations

based on (1) to include the dynamical effects by considering the asymptotic case of a very large dislocation loop. The region enclosed within the loop is a fairly perfect lattice (apart from a stacking fault), the largest distortions being concentrated around the dislocation. The scattered amplitude should therefore be proportional to the length of the dislocation loop rather than to its area as in (1), where $n_c \propto \pi R_c^2$. Also, the scattering on the gradually varying long-range displacement field is overestimated in (1) for scattering with $q < 2\pi/\xi$. In keeping with these considerations and with corrections introduced in standard dynamical theory,[9] the calculation was repeated with (1) replaced by

$$F(\vec{q}+\vec{h}) = n_c(r_c/R_c) j_0(qR_c) \times [(\mp 1 - \Delta V/V) - (\Delta V/V)\vec{q}\cdot\vec{h}q^{-1}s^{-1} - (|\Delta V|/V)\tfrac{1}{3}hr_c], \quad (4)$$

where $s = [q^2 + (2\pi/\xi)^2]^{1/2}$ and $r_c = R_c[1 + (R_c/\xi)^2]^{-1/2}$. The result is shown in Fig. 1(b) for a value of the extinction length ξ, the only adjustable parameter, set to be $\xi = 25$ Å. The comparison with experiment is very satisfactory while for $\xi = 50$ Å it is clearly inferior.

The implication of the present paper is that an electron wave function can adapt adiabatically to gradual lattice distortions for which $|\mathrm{grad}(\vec{g}_i \vec{t}_n)| \ll \xi^{-1}$, giving rise to a distorted trajectory for which the lifetime broadening is greatly reduced. The extinction length gives therefore a simple physical basis for concepts of the minimum effective scattering angle and of dephasing, that have been introduced *ad hoc* to explain conduction-electron scattering on dislocations.[10] A detailed discussion will be published elsewhere.

IV. SUMMARY

The scattering of a conduction-electron Bloch wave on a small lattice defect can be successfully described within the first Born approximation with ion displacements as the perturbation. A numerical calculation without adjustable parameters describes both magnitude and anisotropy of the scattering rate correctly. This scattering corresponds closely to Huang scattering of x rays or neutrons.

For extended lattice defects, the first Born approximation fails since it does not take into account the modification of the Bloch wave within the distorted region of the lattice. Scattering between such modified Bloch waves is reduced compared to the first Born approximation when the lattice distortions are gradual on the scale of an extinction length ξ. The extinction length is a characteristic length for the adaptability of Bloch waves. Introduced in analogy with dynamical scattering theory, ξ is inversely proportional to the lattice potential. An averaged value for electrons in Al, $\bar{\xi} = 25$ Å, has been obtained both from a theoretical estimate and from a fit to the experimental data.

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