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Evaluation of the Threshold Energy for Atomic Displacements in Titanium[†]

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Experimental values of damage rates have been obtained for titanium for electron irradiations in the energy range 0.30–0.50 MeV. A suitable preirradiation annealing treatment has been found, and a value of 19.2 ± 1.0 eV is determined for the threshold energy of atomic displacement for titanium. Experimental damage rates are compared to theoretical calculations of the cross section for atomic displacements.

Two recent publications^{1,2} have treated radiation damage of titanium, but no study has been performed near the characteristic value of the threshold energy for an atomic displacement. While one paper¹ used a theoretical function to extrapolate to a threshold energy value, the other² did not report damage-rate data. This paper describes the dependence of the damage rate of titanium samples on electron-irradiation energy for the energy range 0.30–0.50 MeV. With this information, a reliable value of the threshold energy is estimated and a simple theoretical analysis of the damage-rate curve is made.

Sample material in the form of a thin foil (0.0025 cm) was obtained from Materials Research Corporation. Its nominal purity was 99.97%. However, the natural strong gettering action of titanium can seriously degrade its purity, and the optimum annealing treatment of the material prior to irradiation is therefore of great importance. Before a high-temperature annealing treatment was determined for this titanium, damage rates were investigated for samples annealed at three different temperatures. Most samples showed excessively large damage rates during the first part of an irradiation before the rate became constant and conformed to a linear-flux-versus-damage-rate behavior. Material annealed at 800 °C in a vacuum of 5×10^{-7} Torr was the least reliable since its damage rate values included large fluctuations. Because samples annealed at 350 and 450 °C in a vacuum of 2×10^{-7} Torr gave consistent results for values of damage rate, these samples were used for a determination of the

threshold energy. After samples were mounted in a cryostat, the ratios of electrical resistivity at room temperature (293 K) to that at 7 K were determined. Samples annealed at 450 °C showed values of the resistivity ratio between 10 and 15. For a sample annealed at 350 °C, this ratio was approximately 54. While these magnitudes of the resistivity ratio are not as large as desired for pure sample material, the values are definitely an improvement over titanium samples of other investigators. Because the effects of the preirradiation treatment of titanium is a complex problem, a detailed report on these effects is being prepared.³

At each irradiation energy, the change of electrical resistivity was plotted as a function of fluence. Typical results for one sample are shown in Fig. 1 where the points correspond to experimentally measured values. A large initial damage rate can be seen for each irradiation energy. Because of this initial nonlinear behavior, the first measured value of damage rate was used as a starting point to calculate slopes. The slope was found between each two successive measurements, and an average of these values was taken to represent the damage rate at a particular energy. It is probable that impurities within the material are responsible for the initial excessive damage, and discarding the portion of the curve near the origin helps to ensure that these results concern intrinsic properties of the material.

Figure 2 shows the damage-rate data and theoretical curves for all samples as a function of maximum atomic recoil energy. Since the magnitude

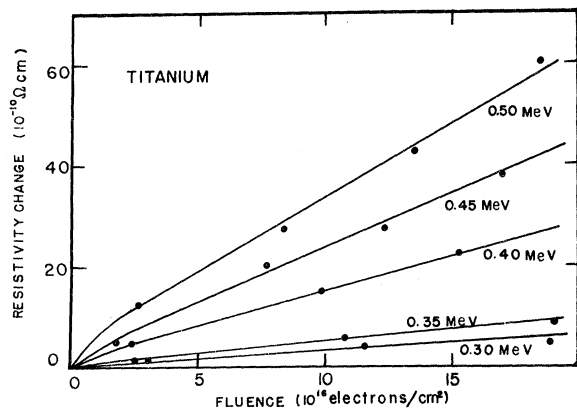


FIG. 1. Changes in resistivity vs fluence for a typical sample.

of the damage rate is very small at the lowest irradiation energy, and since a measurable amount of resistivity change may be caused by impurities, the threshold energy is determined by a straight-line extrapolation (not shown in the figure) of the highest energy values. This procedure gives a resultant value of 19.2 ± 1.0 eV for the threshold en-

ergy for displacing atoms in titanium.

Experimental results may be compared to radiation-damage theory by using the equation

$$\Delta\rho/\Delta\phi = \sigma_d \rho_F,$$

where $\Delta\rho/\Delta\phi$ is the damage rate at a given irradiation energy, σ_d is the cross section for atomic displacements for the irradiation energy, and ρ_F is the resistivity of a unit concentration of Frenkel pairs. The cross section is evaluated by choosing a probability function $P(T)$ for the equation

$$\sigma_d = \int P(T) \frac{d\sigma}{dT} dT,$$

where $d\sigma/dT$ is the differential cross section for an atomic displacement with respect to the atomic recoil energy.⁴ The function $P(T)$ is the probability for displacing an atom with a recoil kinetic energy T . To fit a theoretical curve to the experimental points, two $P(T)$ functions were tried: a simple step function and a linear function.⁵ Figure 2 compares these theoretical results with the experimental data by plotting damage rate versus the maximum atomic recoil energy. Theoretical curves were normalized by selecting a value of ρ_F such that the

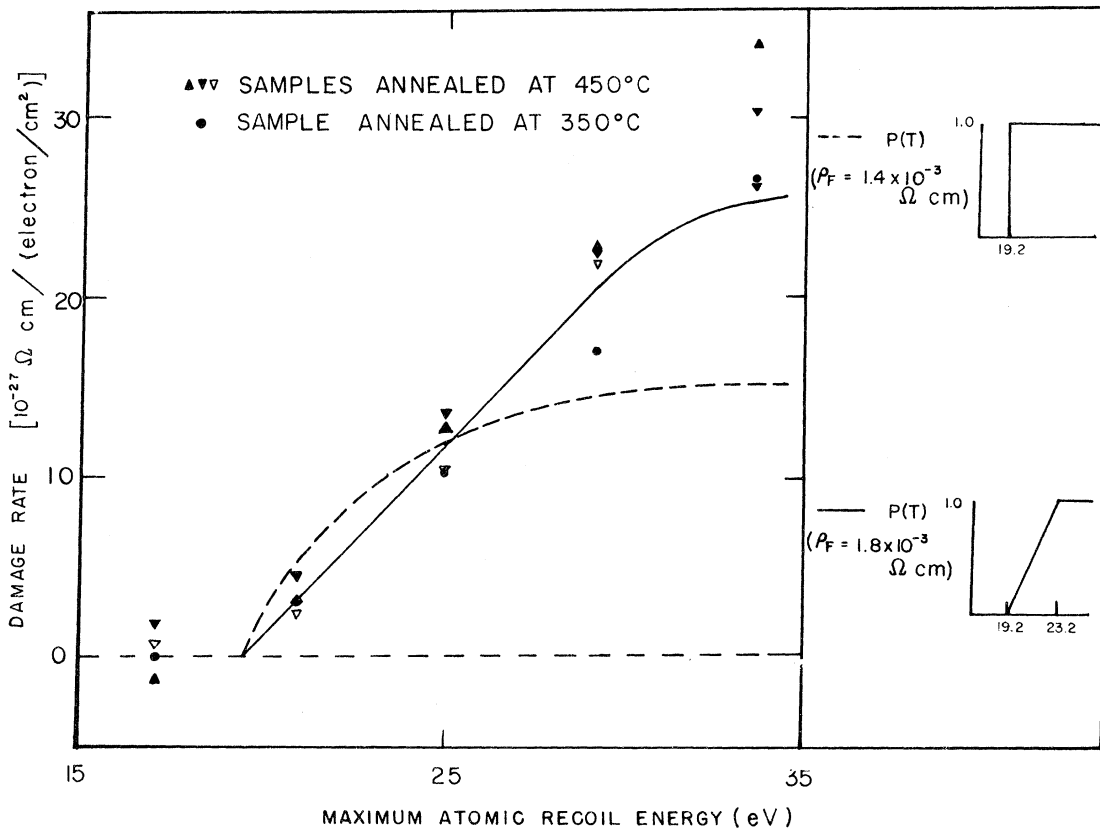


FIG. 2. Experimental results of damage rates for titanium samples and a comparison of theoretical damage-rate curves with experimental data.

curves would coincide with the experimental curve at 24.9 eV, i. e., the maximum atomic recoil energy which corresponds to an 0.4-MeV irradiation. The step function, it is clear from the figure, provides a very poor fit. However, the linear func-

tion departs from the experimental graph only at the highest energies. As with other metals, the poor agreement of the simple step function probably indicates that atoms in the bulk material should be described in terms of an anisotropic function.⁵

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¹P. G. Lucasson and R. M. Walker, Phys. Rev. **127**, 485 (1962).

²W. Bauer, K. Herschback, and J. J. Jackson, Phys. Rev. **185**, 924 (1969).

³G. R. Fletcher (unpublished).

⁴W. A. McKinley and H. Feshback, Phys. Rev. **74**, 1759 (1948).

⁵A. Sosin and W. Bauer, *Studies in Radiation Effects in Solids*, edited by G. J. Dienes (Gordon and Breach, New York, 1969).

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Galvanomagnetic Studies of Bismuth Films in the Quantum-Size-Effect Region*

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Bismuth films (200–1400 Å) were grown epitaxially on freshly cleaved mica substrates. These films consisted of a mosaic of equally oriented crystallites averaging several microns in diameter. The plane of the films coincided with the trigonal plane of Bi. We have studied the thickness dependence of the resistivity, the Hall coefficient, and the transverse magnetoresistance, by gradually varying the thickness of a single film which was kept under high vacuum during the entire experiment. The resistivity at 360 and 77°K is a smooth monotonic function of the thickness. At 12°K, we observed small oscillations in the resistivity and in the magnetoresistance. These oscillations are regarded as probable manifestations of the quantum size effect (QSE). The thickness dependence of the Hall coefficient is in striking disagreement with the predictions of the infinite-potential-well model. Better agreement between the theory and experimental results is obtained when we assume a less rigid boundary condition. Also for several films we have investigated the temperature dependence of these three transport coefficients and found it to be quite different from that of bulk bismuth. We have attempted to explain these results in terms of the behavior of the carrier concentration and of the different scattering mechanisms that can come into play in these films.

I. INTRODUCTION

There are two types of size effect in thin metallic films, each one characterized by a specific parameter. The classical size effect, which has been the subject of numerous investigations, appears in solids whose thickness is comparable to the electron-transport mean-free path. Recently, the quantum size effect (QSE) has aroused considerable interest; it appears when the sample thickness is comparable to the de Broglie wavelength of the conduction electrons. The QSE manifests itself in the oscillatory behavior of the elec-

tron density of states. These oscillations can be observed in the thermodynamic properties and the kinetic coefficients of the solid when the thickness of the film is varied continuously.

In principle, the QSE can be observed in any metal. In practice, the experimental observation in most solids is rather difficult because the electronic de Broglie wavelength is only of the order of a few angstroms. In Bi, however, the Fermi energy of the electrons is only 25 meV, and the effective mass along some crystal orientations is two or three orders of magnitude smaller than the free-electron mass. Consequently, the electronic