Temperature dependence of some structures in electron transmission spectra of Xe solid films

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We report on the temperature dependence of the 3–7-eV structures in the electron transmission spectra of solid Xe films (600 Å). These spectral features are related to the structure factor. We observed an irreversible process consisting of a disorder-order transformation and a reversible process characterized by a Debye-Waller factor $e^{-T/\Theta}$.

In recent papers,[1,2] we studied electron transmission (0–15 eV) through Xe and Kr solid films (0–3000 Å) deposited on platinum polycrystalline foil. Attempts have been made to correlate structures in current-versus-energy plots of the transmitted current with specific electron-target interactions. One of the mechanism that received much interest is interference effects related to the energy dependence of the structure factor. We report here the first electron transmission results where the spectral features of the current-versus-energy plots are clearly related to the structural and thermal order of the thin solid film. The present results were recorded in Xe solid films 600 Å thick using a high-resolution spectrometer.[1,3] The range of temperature we used is 18 to 45 K. Actually 18 K is the minimum temperature we can reach under the conditions of the experiment and 45 K is the maximum at the base pressure 10^{-10} Torr without desorbing the films. The purity of Xe was better than 99.995%.

Figure 1 shows a typical result of electron transmission spectra at measured (T_e) and deposited (T_d)

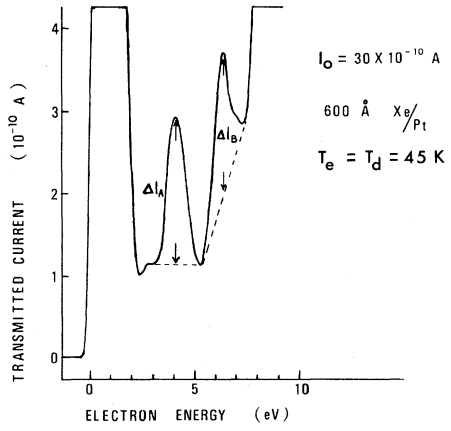

FIG. 1. A typical current-vs-energy plot of the transmitted current through a 600-Å-thick Xe solid film deposited on a clean platinum polycrystalline foil. T_d and T_e are the temperatures of the positions and measurements, respectively. The primary current was 30×10^{-10} A.

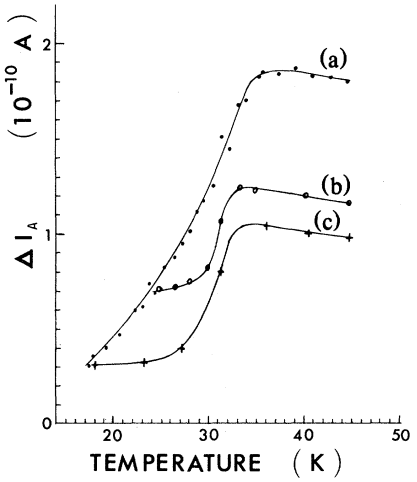

FIG. 2. Temperature dependence of the structure ΔI_A (see Fig. 1): (a) $T_d = T_e = 18$–45 K; (b) $T_d = 25$ K, $T_e = 18$–45 K; and (c) $T_d = 18$ K, $T_e = 18$–45 K.

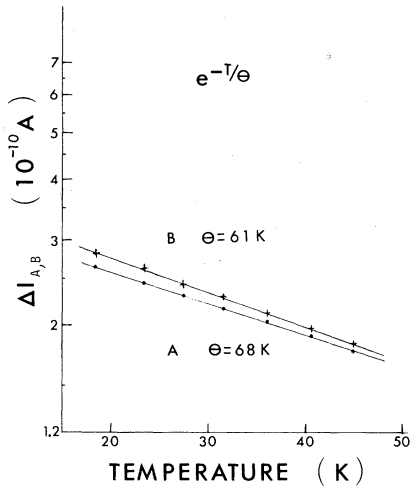

FIG. 3. Temperature dependence of structures ΔI_A and ΔI_B (see Fig. 1) when the film is deposited at 45 K and the current measured from 45 to 18 K (and inversely).

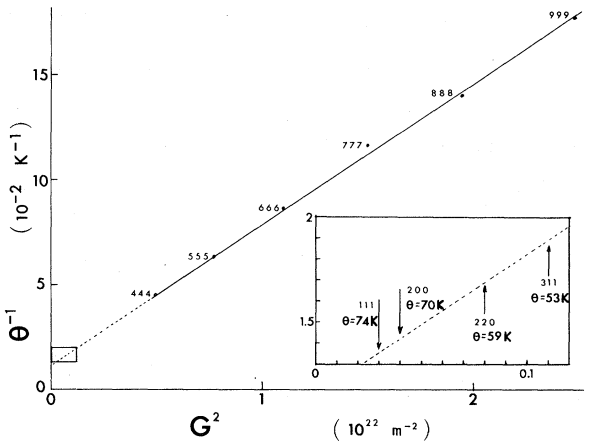

FIG. 4. From the experimental results of Ignatiev and Rhodin (Fig. 12 of Ref. 5) we have calculated and plotted the value $1/\Theta$ of the Debye-Waller factor $e^{-T/\Theta}$ as a function of the square of a reciprocal-lattice vector G for a fcc lattice ($a = 6.17$ Å). The dashed line is an extrapolation of their results.

temperatures of 45 K. In the region 0–8 eV where only elastic processes take place (if we neglect the electron-phonon interaction[1,4]), two large structures around 4 and 6 eV appear. The intensity of those structures ΔI_A and ΔI_B vary as a function of T_e and T_d.

Three different types of experiments can be done: (1) Deposit films at low temperature and measure from low to high temperature (see curves b and c in Fig. 2). (2) Deposit films at high temperature and measure from high to low temperature and inversely (see Fig. 3). (3) Deposit films and measure at the same temperature for different temperatures between 18 to 45 K (see curve a in Fig. 2).

Irreversible processes arose when T_e is increased above T_d (Fig. 2, curves b and c). ΔI_A (and ΔI_B) increased abruptly around 30 K by increasing T_e. This is a typical structural irreversible reordering effect. A resistance to thermal reordering of the first few monolayers at the film metal interface can explain the fact that the curves a, b, and c in Fig. 2 do not end up at the same point at 45 K. This is a memory effect dependent on the conditions of deposition. Indeed, the order at the film metal interface depends on the nature of the interaction between Xe and the metal substrate, the surface of the substrate and T_d. Reversible processes were observed when T_e was maintained below T_d (Fig. 3). ΔI_A and ΔI_B increased (decreased) very smoothly by lowering (increasing) T_e below T_d. The functional variations were characteristic of a Debye-Waller factor $e^{-T/\Theta}$. The deduced values $\Theta_A = 68$ K and $\Theta_B = 61$ K are consistent with the previous low-energy-electron-diffraction (LEED) experiment of Ignatiev and Rhodin.[5] Similar values of Θ can be extrapolated from their results for the Debye-Waller factor of the first Bragg peaks (see Fig. 4).

From a theoretical point of view, the transmitted intensity is inversely poroportional to the cross section at large thickness (600 Å and higher).[1,6] In the independent t-matrix limit, this cross section is related to the structure factor through the relation[1,7]:

$$\frac{d\sigma_s}{d\Omega} = \frac{d\sigma_{\text{eff}}}{d\Omega} S(\vec{k},k') \ ,$$

where $d\sigma_s/d\Omega$, $d\sigma_{\text{eff}}/d\Omega$, and $S(\vec{k},k')$ are the differential cross section for the solid, the effective differential cross section for the atoms, and the structure factor of the solid, respectively. It can be shown that if σ_{eff} is isotropic, we can write

$$\sigma_s(k) = \sigma_{\text{eff}}(k) K(k) \ ,$$

where $K(k)$ has maxima at $k = G/2$ for a well-ordered crystal ($\vec{G}$ is a reciprocal-lattice vector). These maxima in K correspond to the minima in the transmitted intensity. The variation in temperature (T_e and T_d) of ΔI_A and ΔI_B is directly related to the variation in temperature of the structure factor.

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