ERRATA

Roughening of Stepped Metal Surfaces. MARCEL DEN NIJS, EBERHARD K. RIEDEL, E. H. CONRAD, and T. ENGEL [Phys. Rev. Lett. 55, 1689 (1985)].

The main results of the Letter[1] remain unchanged: Stepped metal surfaces [such as the $(11m)$ high-index faces of Cu or Ni] exhibit roughening phenomena well below bulk melting, and such phenomena can be quantitatively explored by the newest atom-beam diffraction techniques. However, an error occurred in extraction of the roughness parameter from the atom-beam diffraction line shapes, which led to incorrect estimates for the roughening transition temperatures T_R of Ni and Cu $(11m)$ surfaces. The correct interpretation gives substantially higher values: $T_R = 450 \pm 50$ K for Ni(115) and $T_R = 730 \pm 50$ K for Ni(113). Ni(001) does not roughen for $T < 1300$ K. With the assumption that the T_R of different materials scale roughly with the bulk melting temperatures, we conjecture that the Cu (115) and (113) faces roughen at $T_R = 350 \pm 40$ K and $T_R = 570 \pm 40$ K, respectively.[2] Therefore, the experiment confirms that the roughening of these metal surfaces takes place in the temperature range suggested by Villain, Grempel, and Lapujoulade.[3]

For $T > T_R$, the diffraction line shapes are predicted to decay as inverse power laws with an exponent governed by the roughness parameter $x_1(T,m)$, which is defined in Eq. (1) of Ref. 1. A mistake in the coordinate transformation from the (001) to the $(11m)$ face led us erroneously to identify (in Fig. 3 of Ref. 1) the experimentally determined roughness parameter with x_1 rather than $\tilde{x}_1 = (m/2)^2 x_1(T,m)$, m odd. (For details see Conrad *et al.*[4]) When T approaches T_R from above, the latter parameter assumes the universal value $\tilde{x}_1^{(R)} = \frac{1}{2}$ for all m. This provides a convenient criterion for the identification of T_R from experiment. For example, the x_1 data for Ni(115) in Fig. 3 of Ref. 1 imply $T_R \approx 450$ K.

For $T < T_R$, the diffraction line shapes are predicted to be Lorentzian. The linear behavior of $\tilde{x}_1$ versus temperature in Fig. 3 of Ref. 1 for $T < T_R < 450$ K seems in disagreement with that prediction, in that it indicates that the line shape can be fitted by an inverse power law even at low temperatures. The new, higher estimate for T_R requires a reanalysis of the effects of inelastic scattering on the diffraction line shapes. A study of those effects for Ni(001),[5] which does not roughen below 1300 K, allows quantitative statements regarding the inelastic contributions to the line shape of Ni(115). We find that, even though one-phonon contributions can be made small for $T > T_R$ (by working at a low-order anti-Bragg angle), inelastic scattering seriously distorts the elastic line shapes for $T < T_R$. The result is that the superposition of the one-phonon corrections and the Lorentzian yields a line shape decaying as an inverse power law with an effective exponent $\tilde{x}_1^{\text{eff}}$ that varies approximately linearly with temperature in $0 < \tilde{x}_1^{\text{eff}} < \frac{1}{2}$. (For details see Ref. 4, Erratum, and Ref. 5.) This explains the linear behavior of $\tilde{x}_1$ versus temperature for $\tilde{x}_1 < \frac{1}{2}$ in Fig. 3 of Ref. 1. Moreover, this effective temperature behavior masked the original error in the coordinate transformation.

The analysis of the diffraction line shape including inelastic correction leads to the experimental result for the roughness parameter $\tilde{x}_1$ of Ni(115) shown in Fig. 1 and gives a value of $T_R = 450 \pm 50$ K. The results are consistent with $\tilde{x}_1 = \frac{1}{2}(T/T_R) + \ldots$ for $T > T_R$ (see Ref. 6) and $\tilde{x}_1 = 0$ for $T < T_R$. For Ni(113) similar behavior has been observed with $T_R = 730 \pm 50$ K.[7]

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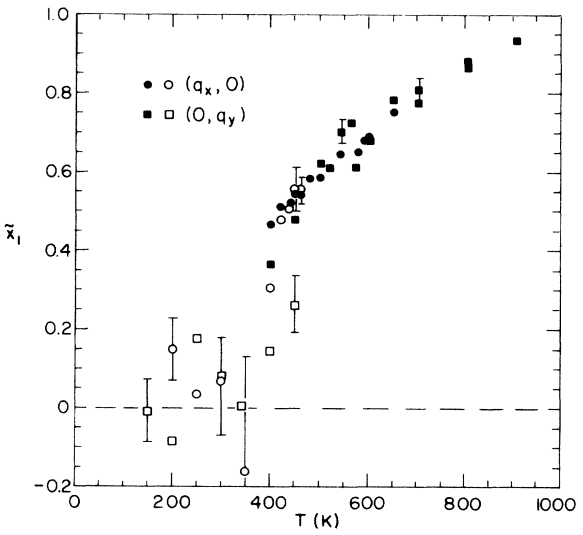

FIG. 1. Roughness parameter $\tilde{x}_1$ vs temperature for Ni(115) from line-shape analysis of the specular peak close to the second anti-Bragg angle, $Q = 3$, for scattering perpendicular (circles) and parallel (squares) to the direction of the steps. Filled symbols are experimental data derived from peak profiles. Open symbols are calculated from peak profiles after the inelastic contributions to the scattered intensity have been subtracted.