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MASTER

SOME ANALYTICAL SOLUTIONS TO THE TWO ATOM BLOCKING MODEL

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Abstract

The two atom blocking model with thermal displacements has been reinvestigated and some new analytical results have been found. For Coulomb scattering, an exact solution for the blocking pattern is found which depends on only two parameters. For scattering from a Moliere potential, a similar parameterization produces a nearly universal set of curves. The results should be useful in analyzing data of ion backscattering experiments that measure crystal surface relaxation.

Recently, Rutherford backscattering has been shown to be a powerful experimental tool for investigating the surface structure of single crystals /1-5/. For instance, two methods have been developed to measure atomic surface relaxation. The first method /1,3,5/ uses an ion beam incident along a channeling direction and the number of target atoms contributing to the backscattering surface peak is measured. The surface relaxation can be deduced from the surface peak because surface relaxation changes the shadow cone that a surface atom casts on its interior neighbor. The second method /4/ uses a combination of channeling and blocking in a double-alignment configuration.

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In this method, surface relaxation manifests itself by an angular shift of the surface blocking pattern in the back-scattered beam.

If such experiments are to give unambiguous surface information, it is important that only a very few atomic layers contribute to the backscattering. Therefore, the two atom blocking model /6/ (developed several years ago for bulk crystal blocking phenomena) should be applicable in analyzing the results from such experiments. Not only is the model directly applicable for interpreting the surface blocking pattern of the second method above, but it can also be used to analyze the surface peak in the first method because of the rule of reversibility /7/. These experiments stimulated a reinvestigation of the model and some new analytical solutions were found which are exact within the framework of classical scattering theory and the impulse approximation.

In the two atom blocking model /6/, a projectile of energy E is emitted (backscattered) from an atomic nucleus at a small angle ψ with respect to the neighboring atom. The projectile is scattered by the neighboring atom through an angle ϕ such that it now moves at an angle θ , which for small angles becomes

$$\theta = \psi + \phi = \frac{S}{l} + \phi(s),$$

where S is the impact parameter and l is the distance between the two atoms. For stationary atoms the normalized differential scattering cross section per steradian is

$$F(\theta) = \frac{1}{l^2} \frac{S}{\theta} \left| \frac{dS}{d\theta} \right| = \frac{1}{1 + \frac{l\phi}{S}} \left| \frac{1}{1 + \frac{l\phi}{S}} \right| \quad \theta \geq \theta_{crit}$$

$$= 0 \quad \theta < \theta_{crit}$$

Here θ_{crit} is the critical angle (minimum of Eq.1). When thermal vibrations are included by using a Gaussian distribution of the relative transverse displacement (mean square amplitude $= \rho^2$) of the emitting and scattering atoms, the emission intensity becomes /8/

$$F(\theta) = \int_0^{\infty} \frac{2s ds}{\rho^2} I_0 \left(\frac{2\ell\theta[s+\ell\phi(s)]}{\rho^2} \right) \exp \left\{ - \frac{[s+\ell\phi(s)]^2 + (\ell\theta)^2}{\rho^2} \right\}, \quad (3)$$

where $I_0(x)$ is the modified Bessel function of the first kind.

In our previous work /6/, Eq.3 was evaluated numerically. However, for a Coulomb potential an exact analytical solution /9/ is

$$F(\theta) = \frac{\beta^2}{2} \exp \left\{ - \left(\alpha^2 + \frac{\beta^2}{2} \right) \right\} \sum_{k=0}^{\infty} \left(\frac{\alpha\beta}{2} \right)^{2k} \frac{1}{(k!)^2} \sum_{r=0}^{2k} \frac{(2k)!}{(2k-r)!r!} K_{r+1-k} \left(\frac{\beta^2}{2} \right). \quad (4)$$

Here $K_r(s)$ is the modified Bessel function of the third kind, $\alpha = \ell\theta/\rho$, and $\beta = \ell\theta_c/\rho$. The quantity $\theta_c = 2\sqrt{Z_1 Z_2 e^2 / \ell E}$ is the critical blocking angle (minimum of Eq. 1) for Coulomb scattering. Equation 4 shows the explicit dependence of the emission intensity $F(\theta)$ on two parameters, α and β , whereas the original problem contains six parameters, $z_1, z_2, E, \ell, \rho, \theta$. A complete solution can be displayed, therefore, by a single set of contour lines as shown in Fig. 1. These numerical results were obtained using a computer and are accurate to about 0.1%. From this universal plot, a blocking pattern for any particular case may be easily constructed. First, draw a vertical line corresponding to the β value of interest, and then read off the values of α at those points where the vertical line intersects the contour lines. For the special case $\theta = 0$, Eq.4 reduces to a single term such that the emission intensity $F(\theta)$ is a function of a single parameter,

$$F(0) = \frac{\beta^2}{2} \exp \left(- \frac{\beta^2}{2} \right) K_1 \left(\frac{\beta^2}{2} \right) \quad (5)$$

For large values of β (corresponding to small thermal displacements, for instance) Eq.5 predicts $F(0) \approx 0$ or complete blocking, as expected. On the other hand, for small β (large ρ) $F(0) \approx 1$, which again is expected as the shadow cone then disappears.

For scattering from a screened Coulomb potential, such as the Molière potential, an analytical solution to Eq.3 appears difficult. With such a potential, there is the additional parameter describing the screening distance. However, the Coulomb results suggest that a similar parameterization, in which the Coulomb critical angle is replaced by the Molière critical angle, may work. Therefore Eq.3 was computer evaluated for a large number of cases. Figure 2 shows that a fairly universal set of curves is obtained over a wide range of parameter values. To construct a blocking pattern from these curves, one needs to know the Molière critical angle, which is more difficult to calculate than the Coulomb case. The ratio of the Molière critical angle to the Coulomb critical angle however, can be shown to be a function of single parameter, $\frac{l}{a}\theta_c$, where a is the screening distance. This ratio has been calculated and plotted in Fig.3. From Fig.3 one can determine the Molière critical angle for any particular case and then construct the corresponding blocking pattern from Fig.2 in the manner discussed for the Coulomb case. As an example of the use of the model, Fig.4 shows: 1) measurements of the surface backscattering peak made by Davies et al. to determine the relaxation of the outer atomic layer on the (111) surface of platinum, 2) results of a computer simulation by Barrett, and 3) results of the two atom blocking model. From this figure the magnitude of the relaxation inferred is 0.22 Å. Except at high energies or when the effective number of atoms per row approaches two, the results of the blocking model agree well with the computer simulations which include all of the row atoms. The two atom blocking model results in Fig.4 can be constructed from the universal curves of Figs.2 and 3 as follows: For each assumed outward relaxation distance Δd evaluate $l = d + \Delta d \cos(\gamma)$, where d is the distance between a surface atom and its interior neighbor in the absence of relaxation and γ is the angle between [011] and the surface normal. Next calculate $\theta_c = 2\sqrt{Z_1 Z_2 e^2 / \lambda E}$ and use Fig.3 to get θ_m .

Finally evaluate $\theta = \frac{\Delta d \sin \gamma}{l}$, $\frac{l\theta}{\rho}$, $\frac{l\theta_m}{\rho}$

and read off the values of $F(\theta)$ from Fig.2. The quantity $F(\theta)+1.0$ gives the number of atoms per row contributing to the surface back-

scattering peak (the 1.0 is from the unshadowed surface atom).

In applying the two atom blocking model it should be noted that it is the relative transverse displacement of the two atoms that explicitly enters the formula. In the absence of correlations between the thermal displacement of the two atoms, the mean square relative transverse displacement of the two atoms, the mean square relative transverse displacement is related to the mean square transverse displacement of a single atom by $\rho^2 = 2 \rho_1^2$.

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Figure 1. Universal Emission Intensity Curves of the Two Atom Blocking Model for Coulomb Scattering. $\theta_c = 2\sqrt{Z_1 Z_2 e^2 / \lambda E}$ is the Critical Angle.

Figure 2. Nearly Universal Emission Intensity Curves of the Two Atom Blocking Model for Mollere Scattering. θ_c is the Mollere Critical Angle. Curves calculated using $Z_1=2, Z_2=78, \lambda=2.47\text{\AA}, a=0.11\text{\AA}$.

Fig. 3. Universal Curve for the Ratio of the Moliere Critical Angle to the Coulomb Critical Angle as a Function of the Reduced Variable $\frac{l}{a} \theta_C$.

Effective Number of Atoms per Row Contributing to Backscattering of ^4He Ions Incident Along [011] onto a (111) Pt Surface at 40 K ($P = \sqrt{2} R = 0.061 \text{ \AA}$).