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COMPUTER SIMULATION OF THE GRAZING INCIDENCE BACKSCATTERING OF PROTONS FROM A (110) NICKEL SURFACE

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ABSTRACT

The computer program MARLOWE has been used to study the processes whereby protrons are reflected from the (110) surface of a nickel crystal. The ions were incident in the (001) plane, at an angle of 7.5 degrees from the surface. Energy and angular distributions of the backscattered particles were investigated for the incident energy range 0.1 to 5 kev. The results were compared with similar ones for an amorphous target.

Total reflection of the beam occurred below 1.2 keV. Focusing in the [$1\bar{1}0$] semichannels was found to be energy dependent and to be strongest under total reflection conditions. The energy distributions of the reflected particles showed a complex structure which is dependent on the incident energy. This structure is interpreted in terms of detailed reflection mechanisms.

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[*] Operated by Union Carbide Corporation for ERDA.

Surface analysis by backscattering methods requires a detailed understanding of the ion-surface interaction processes. Much work has been done recently concerning the influence of surface crystallography,(1) impurities,(2) defects(3) and thermal vibrations(4) on the reflection of ions, as well as on charge exchange mechanisms.(5) This paper is concerned with the effects of surface structure on the reflection of light atoms from a nickel target. The computer program MARLOWE, described elsewhere,(6,7,8) was used for a series of simulated experiments.

The target was a single crystal of adjustable thickness, bounded by two parallel (110) planes which defined the surfaces. Provision is made in the computer model for randomization of the structure. When this option is employed, directional correlations are destroyed but the density of the crystal is preserved, thus mimicking an amorphous or liquid-like medium. Calculations have been performed for grazing incidence hydrogen atoms in the energy range from 0.1 to 5 keV. Under such conditions, the energy losses of the incident particles are dominated by inelastic (electron excitation) effects, but their trajectories are controlled by their quasi-elastic scattering from the target atoms. Various particle detectors of adjustable acceptance angle could be located where desired outside the target. The collected atoms were counted and their energy distribution determined.

The quasielastic scattering of the incident H atoms from the target Ni atoms was based on the Molière approximation to the Thomas-Fermi interatomic potential, with the Firsov screening length. The inelastic loss model included an exponential dependence on the apsis in the collisions and normalization to the Lindhard theory for random encounters at high energy.(7) The lattice was static, no thermal displacements being considered.

Figure 1 shows a comparison of the energy distributions calculated for hydrogen atoms reflected from a monocrystalline and from a random target. Enough projectiles of 3 keV initial kinetic energy were employed so that the reflection coefficient was evaluated with a standard deviation of about two percent. The plane of incidence on the monocrystal target was taken parallel to the (001) crystallographic planes, which intersect the surface in the direction of the [1$\bar{1}$0] semichannels. The incident direction made an angle of 7.5 degrees with the (110). A detector of 1 degree acceptance angle was located in the direction corresponding to specular reflection. The monocrystal target contained 12 atomic layers (13.71 Å). The thickness of the amorphous target was 14.1 Å.

Two main differences are evident between the results obtained for the crystalline and the amorphous targets:

1. The number of particles counted in the specular detector is larger when the target is a perfect crystal than when directional correlations are destroyed. Focusing results from the surface crystallinity and will be discussed below.
2. The energy distribution of atoms reflected from an amorphous surface has a single mode corresponding to the "surface peak" and a tail similar to many experimental spectra, while in the single crystal case, several distinct modes occur both for all the reflected particles and for the atoms collected in the specular detector. These can be attributed to distinct reflection mechanisms.

In order to identify such mechanisms, the contributions of each atomic layer to the energy distribution of atoms collected in the specular detector were evaluated. Figure 2 shows the distributions obtained for the first four atomic layers of the target. The peak corresponding to the smallest energy loss in Fig. 1a is due to the specular reflection of the ions from the surface plane only. The next peak includes contributions from the first and second layers. The third peak is due to reflection from the first three layers, the fourth to the third and fourth layers, and the fifth could be attributed to the contribution of the third atomic plane only. While the last was statistically very doubtful, it was observed also at other energies. Deeper layers do not contribute to specular reflection from the crystalline target at this energy. An analysis of the energy lost by the projectiles as a function of their impact points on the surface during specular reflection from the upper atomic layer shows that the peak corresponding to the smallest energy loss in Fig. 1a is due to scattering from one row of atoms. Since binary events are prevented by the incidence conditions, they cannot help to explain any peak. On the other hand, it can be seen that the second and third peaks in the energy distributions from one atomic layer (Fig. 2) correspond respectively to two and three times the energy loss for scattering from one row. They can thus be attributed to reflection after two and three successive interactions with surface rows. Consequently, the specular reflection of protons from a nickel (110) single crystal appears to be the result of the interaction with one, two or three rows from the three first atomic layers. Reflection from a single row in the second layer (the bottom of the semichannels) is the most probable process.

The lower probability of specular reflection from the surface plane than from the plane below it requires special comment, since the [1$\bar{1}$0] rows in both planes are exposed to the incident beam and their contributions might be supposed to be equal. The incident H atoms that are multiply scattered from a single atomic row leave this row at approximately the same angle at which they approach it. If the row lies in the target surface, a portion of the scattered particles will be backscattered without significant interaction with other atoms in the crystal. As a result, the atoms backscattered from a surface row have directions lying on the surface of a cone of half-angle equal to the incident angle. This cone includes the specular detector, but most of the particles lying on it miss this detector. They appear in other regions of the calculated angular distributions. In contrast, atoms backscattered from rows in the second layer, that is from the bases of the semichannels, cannot escape from the crystal without further scattering as they pass the surface rows. This tends to direct them once again into the specular detector.

In order to determine the influence of the incident energy on the energy distributions of the reflected particles, the calculations were repeated at various energies between 0.1 and 5 keV. All five of the peaks in the energy distributions have been observed only for incident energies above 2 keV. At energies lower than about 1 keV, reflection from pairs of surface rows and from single rows in the second layer seemed to be the only processes contributing to specular reflection. Reflection from single surface rows takes place at energies larger than 2 keV and is of increasing relative importance with increasing incident energy. It becomes the dominant mechanisms of specular reflection at about 4.5 keV. As an example, the energy distributions calculated with a 5 keV incident energy are shown in Fig. 3.

Figure 4 shows the energy dependence of the reflection coefficient and of the yield of protons collected in a detector of 1 degree acceptance angle located in the specular direction. In the low energy range, a comparison is also made with the number of particles detected one and two degrees azimuthally from the specular detector, the angle with the surface plane being fixed at 7.5 degrees. The results show evidence of an "energy threshold" for total reflection which corresponds to an incident transverse kinetic energy (energy component normal to the surface) of 23.8 eV. As shown elsewhere(8) for the "angular threshold" of total reflection, at lower transverse kinetic energies, no projectiles penetrate the target. The number of particles collected in the specular detector is a maximum at energies near 1 keV where the reflection coefficient equals unity. Yields in the other detectors are much less dependent on the incident energy. This reveals the focusing of protons in the $[1\bar{1}0]$ semichannels which is the strongest in the 1 keV region. When conditions are reached such that projectiles can penetrate the target, the reflection coefficient is a decreasing function of the incident energy. In the high energy region however, this decrease is partially due to the thinness of the target (6 atomic layers, 6.23 Å).

At 3.2 keV, the reflection coefficient passes through a minimum, which can be explained by the fact that near this energy, particles scattered by surface rows penetrate into the $[1\bar{1}0]$ channels lying just beneath the surface and travel long distances on stable trajectories. Such subsurface channeling of light particles has been discussed by Sizman and

Varelas$^{(9)}$ at higher energies. The minimum in the reflection occurs at an energy such that a significant fraction of the incident atoms (about 10 percent) is scattered to within the critical channeling angle of the [1$\bar{1}$0] (and perhaps [001]) channels which lie just beneath the target surface. At both lower and higher energies than the minimum, a decreasing fraction of particles is scattered within this critical angle. The changing incident atom energy thus causes a portion of the scattered beam to scan across the subsurface channels, so that the structure near 3 keV in Fig. 4 is just a mapping of a conventional channeling minimum, bordered by two maxima as usual.

The aim of these calculations has been to elucidate some of the reflection mechanisms prevailing for low energy light ions under glancing incidence on static monocrystals. The effects on these mechanisms of thermal displacements of the lattice atoms and of surface defects, either chemical or structural, must be investigated. It seems likely that the sensitivities to these factors will be sufficient to allow light ion scattering to be a useful surface structural probe.

REFERENCES

(1) E. S. Mashkova and V. A. Molchanov, Rad. Effects 23, 215 (1974).

(2) W. Heiland and E. Taglauer, J. Vac. Sci. Techn. 9, 620 (1971); Appl. Physics 9, 261 (1976).

(3) W. Heiland and E. Taglauer, Rad. Effects 19, 1 (1973).

(4) B. Poelsema, L. K. Verhey, and A. L. Boers, Surface Sci. 55, 445 (1976); Nucl. Instr. Meth. 132, 623 (1976).

(5) H. Verbeek, W. Eckstein, and S. Datz, J. Appl. Phys. 47, 1785 (1976); W. Eckstein and F. E. P. Matschke, Phys. Rev. B 14, 3231 (1976).

(6) M. T. Robinson and I. M. Torrens, Phys. Rev. B 9, 5008 (1974).

(7) O. S. Oen and M. T. Robinson, Nucl. Instr. Meth. 132, 647 (1976).

(8) M. Hou and M. T. Robinson, Nucl. Instr. Meth. 132, 641 (1976).

(9) R. Sizman and C. Varelas, Nucl. Instr. Meth. 132, 633 (1976).

FIGURE TITLES

Fig. 1. Reflected particle energy loss spectra calculated for 3 keV H atoms incident on Ni targets at a glancing angle of 7.5 degrees. a) A (110) crystalline target of 12 atomic layers (13.71 Å). b) An amorphous target 14.1 Å thick. The inset shows the geometry of the calculations.

Fig. 2. Specular reflected particle energy loss spectra calculated for 3 keV H atoms incident at glancing angle of 7.5 degrees onto (110) Ni targets of various thicknesses.

Fig. 3. Reflected particle energy loss spectra calculated for 5 keV H atoms incident at glancing angles of 7.5 degrees onto a (110) Ni target of 6 layers (6.23 Å).

Fig. 4. The energy dependence of the reflection coefficient calculated for H atoms incident at a glancing angle of 7.5 degrees onto a (110) Ni target of 6 layers (6.23 Å).

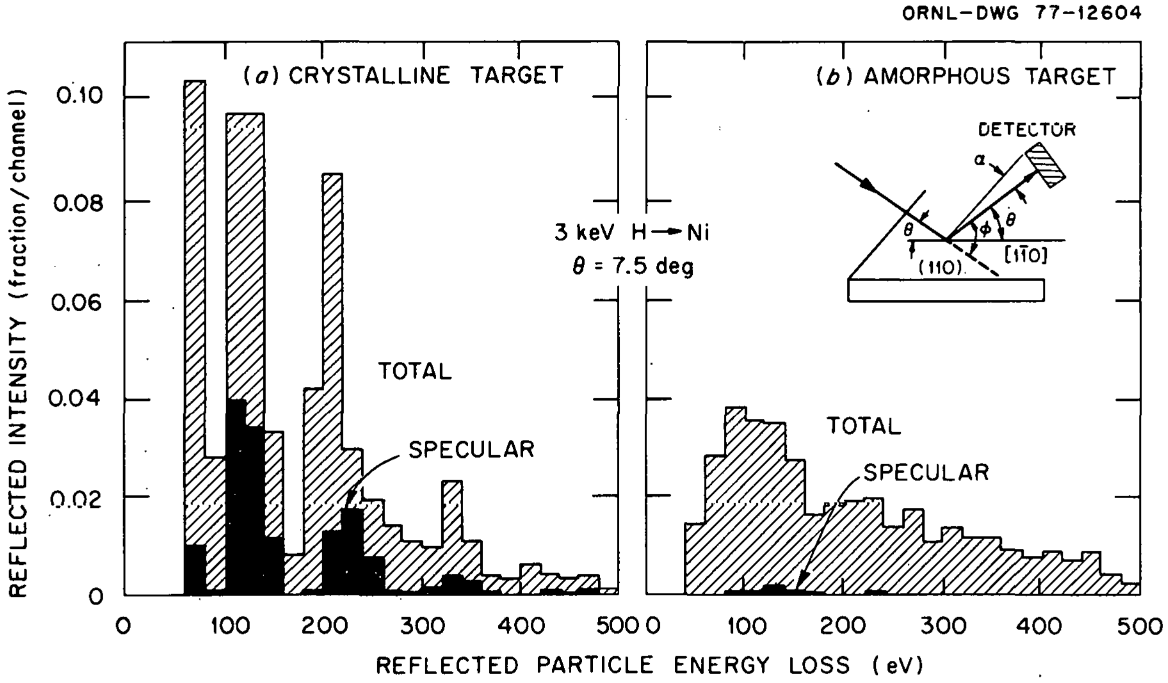
ORNL-DWG 77-12604
(a) CRYSTALLINE TARGET
(b) AMORPHOUS TARGET
REFLECTED INTENSITY (fraction/channel)
0.10
0.08
0.06
0.04
0.02
0
TOTAL
SPECULAR
3 keV H → Ni
θ = 7.5 deg
DETECTOR
α
θ
ϕ
(110)
[1$\bar{1}$0]
0
100
200
300
400
500
REFLECTED PARTICLE ENERGY LOSS (eV)

Fig. 1.

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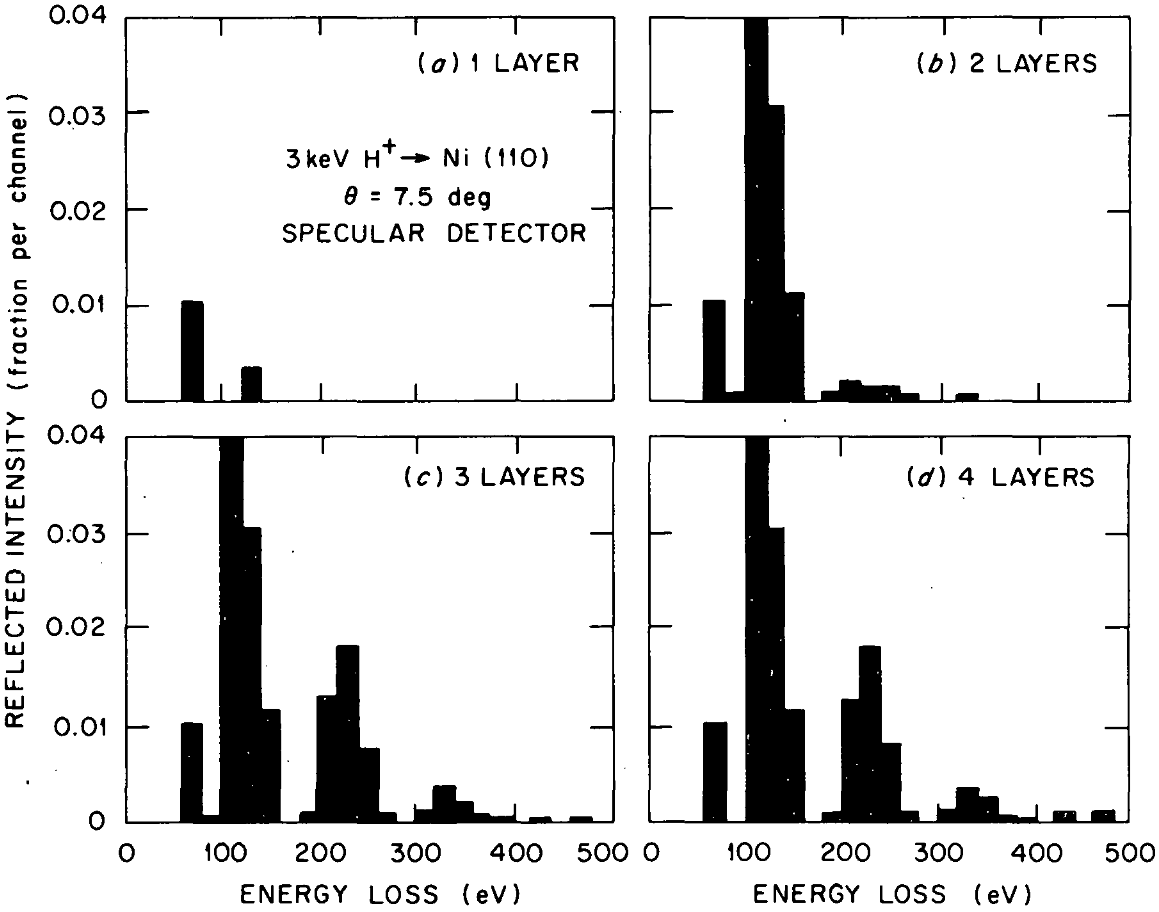

Fig. 2.

ORNL-DWG 77-12602

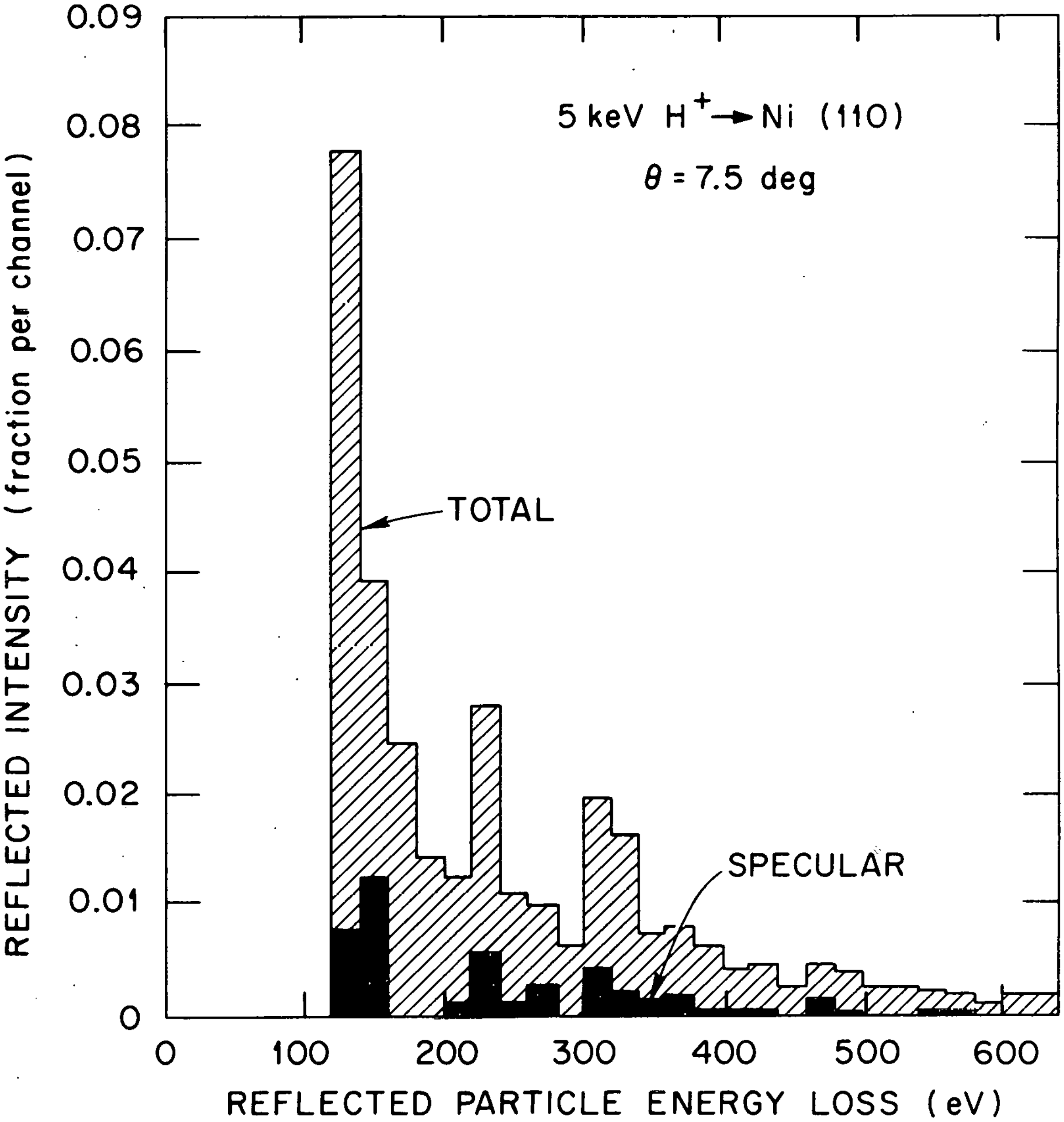

Fig. 3.

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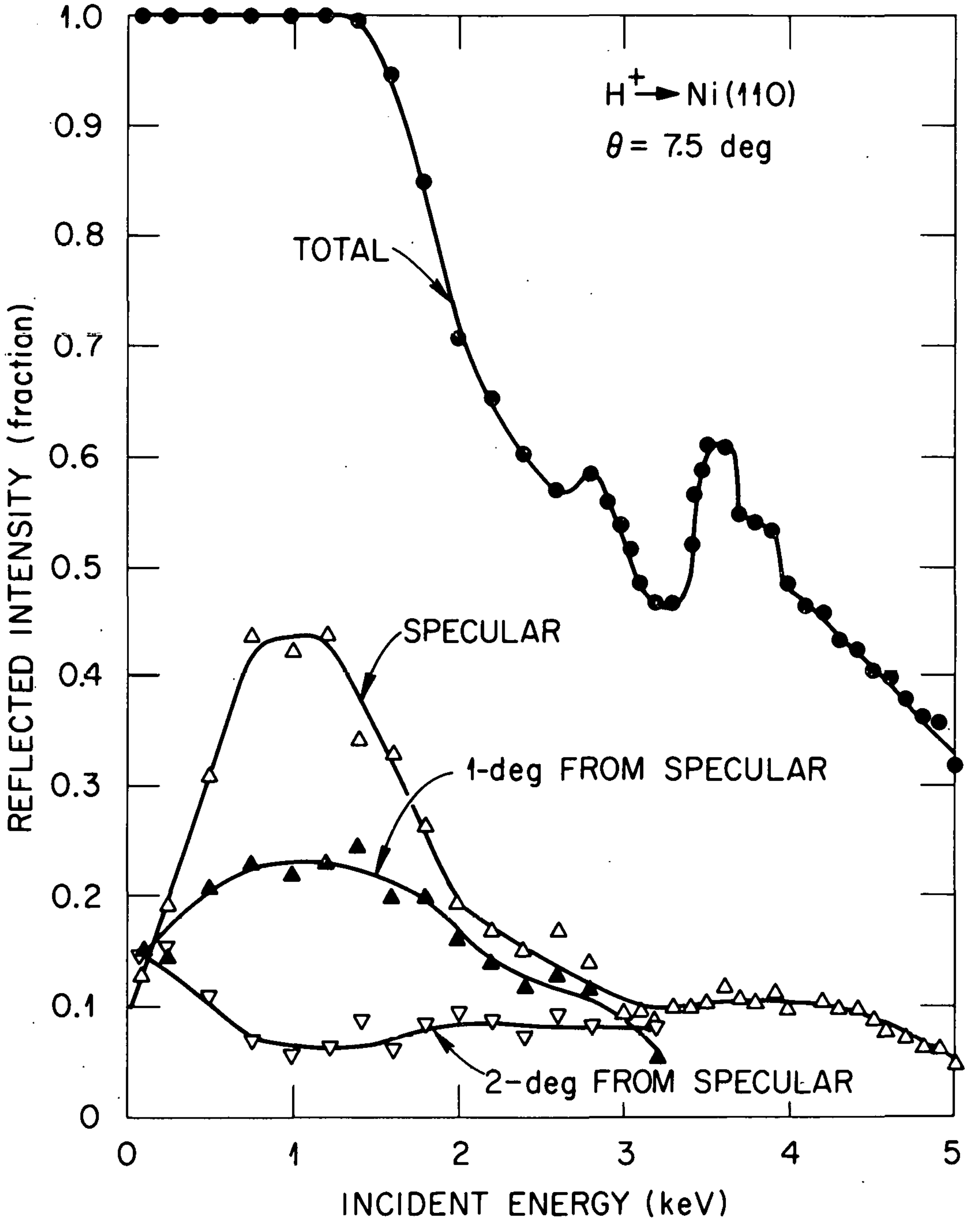

Fig. 4.