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COMPUTER STUDIES OF THE SCATTERING OF LOW ENERGY HYDROGEN IONS FROM POLYCRYSTALLINE SOLIDS

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ABSTRACT

Reflection of 50 eV to 10 keV H atoms from polycrystalline Cu, Nb and Au targets has been calculated using the binary collision cascade program MARLOWE. The fractions of particles and energy reflected (backscattered) increase with increasing atomic number of the target and decrease with increasing incident energy. The results indicate that the effects of polycrystallinity are modest, reducing the amorphous reflection coefficients by about 25%. The calculations agree quite well with the experimental data for Cu and Au, but are about a factor of two larger than is observed for Nb.

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Hydrogen recycling between the walls and the plasma in a controlled thermonuclear reactor can lead to important conseqeunces in the particle and energy balances of the system [1]. The hydrogen ions, through charge exchange, will escape a magnetically confined plasma and bombard the first wall of the containment vessel. A fraction of the hydrogen will be reflected (backscattered) from the walls back into the plasma with reduced energy while the remainder will slow down and come to rest within the walls. For reactor design it is necessary to know the amount and the energy distribution of the reflected hydrogen. Although the backscattering of hydrogen ions with energies above 100 keV has been studied extensively for many years, only a limited amount of experimental [2-6] and theoretical [7-13] work has been done for incident energies of a few keV or less which is the region of most interest to current fusion research. Experimentally, the problem is greatly complicated by the difficulty in detecting the low energy reflected neutral atoms. Previous theoretical studies have treated only the reflection from amorphous targets. Reflection from polycrystalline targets is the subject of the present paper. This is important since most experimental targets possess sufficient crystalline texture to affect the motion of the ion through channeling.

The present work was designed to study the reflection of 50 eV to 10 keV H from polycrystalline solids. The calculations were done using the computer program MARLOWE [14] modified in order to study reflection coefficients [13]. In brief, the projectile ion strikes the target surface and is followed collision by collision in the solid until it either leaves the surface again or until its energy falls below a predetermined value (5 eV). Each collision with a target atom consists of an elastic

and an inelastic part. Only the elastic part, described by a screened coulomb potential, deflects the projectile, whereas energy is lost in each part. The magnitude of the inelastic stopping cross section is chosen to match the electronic stopping theory of Lindhard *et al.* (LSS)[15] above about one keV. There is little experimental information about the electronic stopping of low energy ions, however, recent measurements in Cu, Ag and Au by Nomura and Kiyono [16] using hydrogen ions down to 4 keV agree well with the LSS predictions.

MARLOWE was originally developed to treat monocrystalline solids. Polycrystalline solids are simulated as follows. The single crystal target has a given predetermined surface plane exposed to the incident beam. The incident projectiles are initialized such that they hit randomly with a uniform distribution over a given surface cell. Prior to the first collision the coordinate frame in which the crystal is described is rotated randomly in three dimensions with respect to the fixed frame in which the projectile is moving. Three appropriate Eulerian angles [17] are used in making this rotation. Having selected a particular orientation, the motion therein of a projectile is followed until its history is terminated. The whole process is repeated for each projectile so that in a typical run of a 1000 histories there would be that number of different crystal surfaces exposed. A consequence of this polycrystalline simulation method is that the crystal grain size is larger than the maximum range of the projectile.

An additional feature of the present investigation is the inclusion of thermal vibrations of the target atoms. In our previous studies of amorphous solids their inclusion would have been redundant. However, in a

crystal calculation it is desirable to include them since they affect the degree of channeling. Thermal vibrations are based on a Debye model in which each target atom vibrates independently [14].

The present calculations are for H incident normal to polycrystalline targets of Cu, Nb and Au at T = 293°K with Debye temperatures of 315, 275 and 182°K respectively. The overall results are similar to those reported previously for amorphous targets [13]. Both the fraction of particles and of energy reflected increase with increasing target atomic number and decrease with increasing energy. Some details of the reflection for two incident energies are shown in Fig. 1. As the energy increases from 0.1 to 5 keV the fraction of particles reflected decreases from 0.49 to 0.18 and that of energy from 0.34 to 0.07. Meanwhile the average energy of hydrogen reflected, expressed as a fraction of the incident energy decreases from 0.70 to 0.39. The top histograms show that the peak in the energy distribution of the reflected particles broadens and shifts to lower fractional energy with increasing incident energy. This shift may be understood from the lower histograms which show the maximum penetration depths of those particles reflected. It is seen there that the strong reflection from the surface layers which is present for 0.1 keV incident energy is absent at 5 keV. The angular distributions of reflected particles (middle histogram) are similar for both incident energies and approximate a cosine distribution.

Figure 2 compares the present polycrystalline results with our previous amorphous calculations. The top half of the figure shows the ratio of the amount of hydrogen reflected from the polycrystalline targets to that of their amorphous counterparts as a function of the reduced energy,

ε [15]. Similarly, the ratio of the energy reflected from the two types of targets is shown at the bottom of Fig. 2. These results indicate that the effects of polycrystallinity are modest, reducing the amorphous reflection coefficients by about 25%. It appears that the effects of polycrystallinity are less at low and high energies; however, this point needs further investigation. No specific differences were found between the bcc (Nb) and the fcc (Cu and Au) polycrystalline calculations.

In Fig. 3 the fractions of particles and of energy reflected are plotted against incident energy expressed in reduced units. By using these reduced units a fairly good universal curve is obtained for the reflection of hydrogen in arbitrary target material. It is seen that the deviations from universality indicated by the scatter of the point is comparable in magnitude to the differences between the present calculations and our previous amorhpous results, also shown. Comparing with the experimental results of Andersen *et al.* [5] and of Sidenius and Lensjaer [3], it is seen in Fig. 3 that the calculated fraction of particles agree quite well with the Cu and Au data, but less well with Nb. The calculated fraction of energy reflected is somewhat higher than that observed, especially at the higher energies. Again the poorest agreement is found for Nb targets where the calculated values are about a factor of two greater than observed. There are at least two possible reasons for this: the electronic stopping assumed in the calculations may be too low or oxide layers may be present in the experimental targets which were not included in the calculations. The experimental work done to date is of relatively high energy (> 5 keV) with respect to current fusion needs. Barnett and Ricci [6] are currently making measurements with lower incident energies.

Until experimental information at low energy is available the present calculations can serve as a guide for CTR needs.

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FIGURE TITLES

Fig. 1. Energy, angular, and maximum penetration distributions of hydrogen reflected from polycrystalline niobium. The dashed sloped line in the angular plots is a cosine distribution shown for comparison.

Fig. 2. Ratio of polycrystalline target results to those for amorphous targets for the fraction of particles and energy reflected. The reduced incident energy unit, ε, is defined in Fig. 3.

Fig. 3. Particle and energy reflection coefficients as functions of reduced energy, ε. The incident ion energy in keV is found by multiplying ε by the appropriate scaling factor, E_L.

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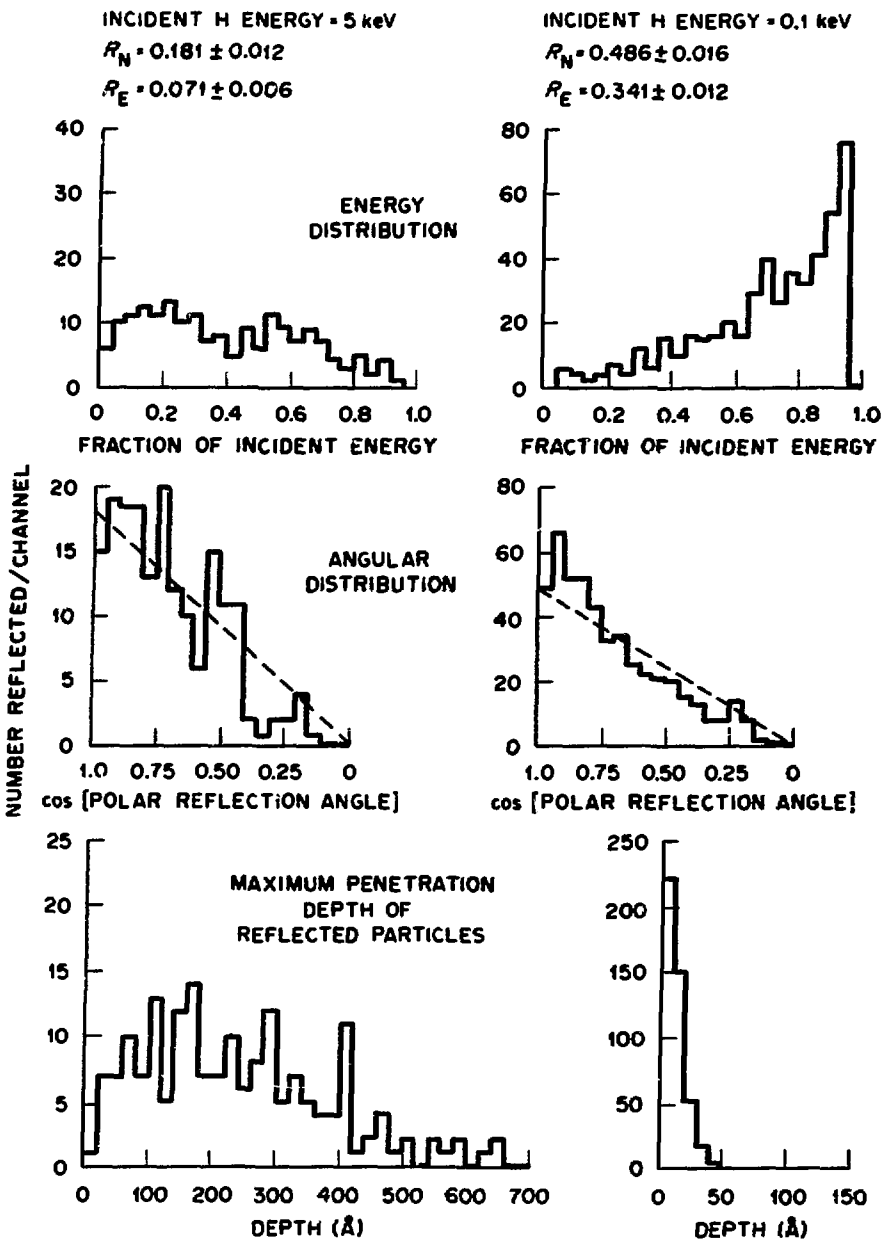
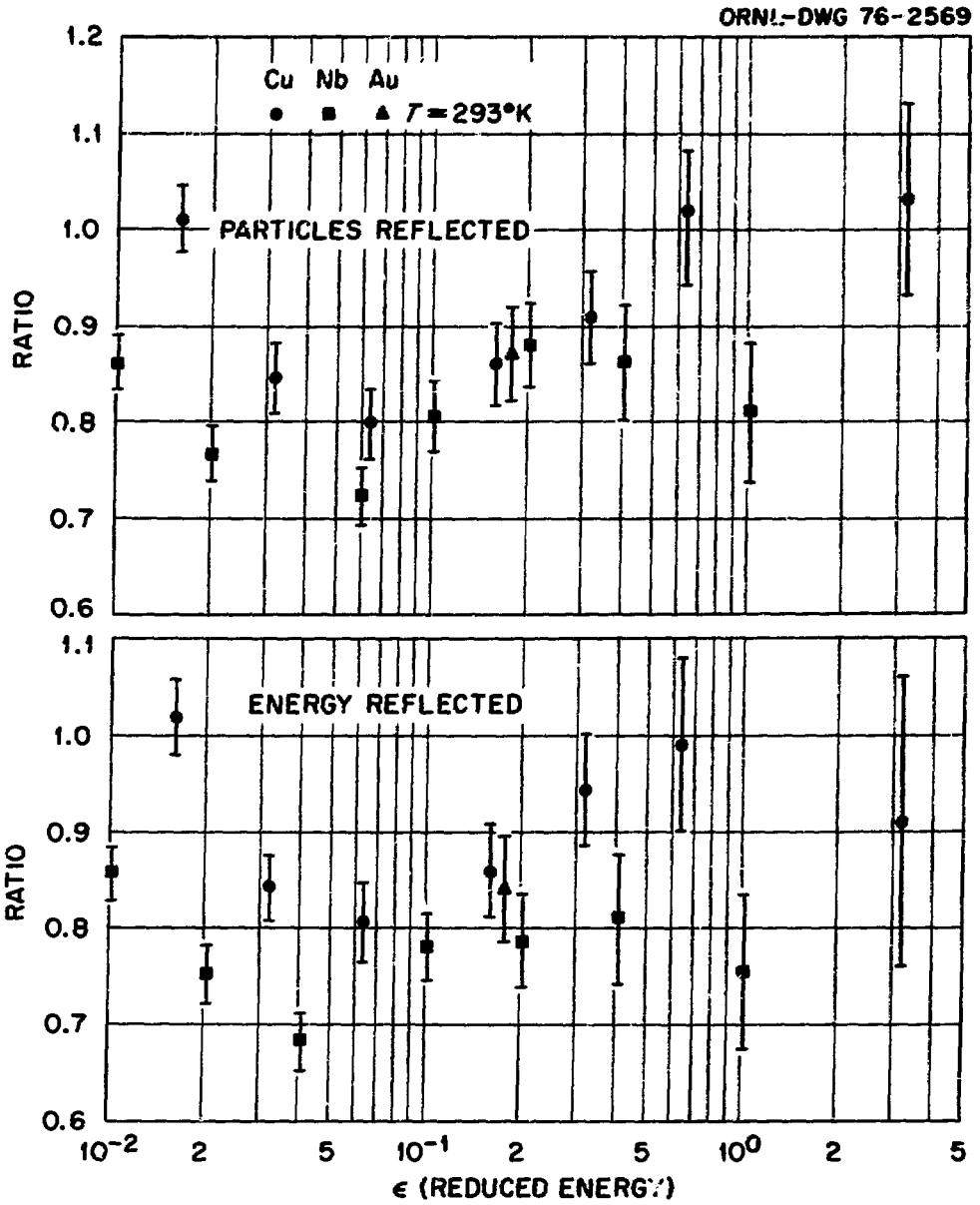


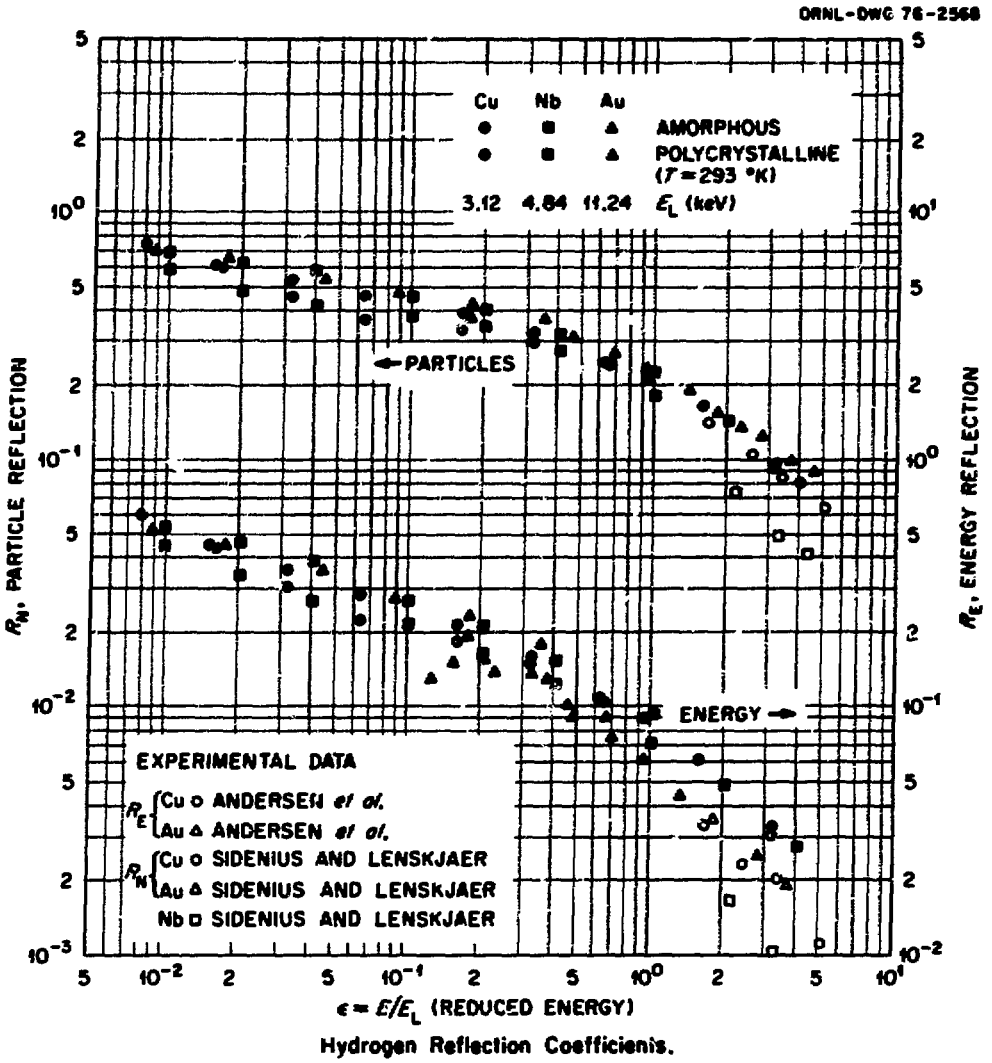
Hydrogen Reflectivity from Polycrystalline Niobium (T = 293 °K)

Fig. 1



Ratio of the Hydrogen Reflectivity of Polycrystalline Targets to that of Amorphous Targets.

Fig. 2



Hydrogen Reflection Coefficients.

Fig. 3