

1976

## Scattering of argon and Neon from W(112)

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### Publication Info

Published in *The Journal of Chemical Physics*, Volume 64, Issue 1, 1976, pages 41-44.

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White, R. E., Ehrhardt, J. J., & Merrill, R. P. (1976). Scattering of Argon and Neon from W(112). *The Journal of Chemical Physics*, 64 (1), 41-44.

<http://dx.doi.org/10.1063/1.431937>

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Citation: *The Journal of Chemical Physics* **64**, 41 (1976); doi: 10.1063/1.431937

View online: <http://dx.doi.org/10.1063/1.431937>

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# Scattering of argon and neon from W(112)

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(Received 27 May 1975)

The angular scattering distributions of thermal Ne and Ar beams incident in the  $[1\bar{1}0]$  azimuth of the W(112) surface are presented as a function of angle of incidence, surface temperature, and beam temperature. For Ne, the distributions are rainbow patterns similar to those observed for Ne on LiF for small angles of incidence. They coalesce into a broad lobe at an incidence angle of  $70^\circ$ . Argon scattering is unilobular and similar in all details with Ar scattering from the smoother W(110) surface. Ne appears to be in the inelastic regime while Ar is trapping dominated.

## INTRODUCTION

The scattering of rare gases from relatively smooth metal surfaces typified by fcc (111), fcc (100), and bcc (110) have been studied extensively.<sup>1-4</sup> These surfaces produce only unilobular scattering. By contrast, He, H, H<sub>2</sub>, and D<sub>2</sub> scattering from the strongly periodic surfaces of alkali halides (principally LiF) shows diffraction.<sup>5-7</sup> Thermal Ne beams from LiF exhibit two broad rainbow peaks,<sup>3</sup> i. e., one forward scattered from the specular angle and one backward scattered, while monoenergetic Ne beams show diffraction.<sup>9</sup>

Tendulkar and Stickney<sup>10</sup> demonstrated that the periodicity of W(112) in the  $[1\bar{1}0]$  azimuth is strong enough to diffract He, and it has been shown in this laboratory<sup>11</sup> that W(112) produces rainbow scattering of thermal Ne beams. In this paper scattering patterns of Ne and Ar from W(112) are presented as a function of gas temperature, surface temperature, and angle of incidence. Similar data for He scattering are presented in a companion paper.<sup>12</sup>

The surface structure of W(112) in the  $[1\bar{1}0]$  direction consists of ridges of close-packed tungsten atoms 4.47 Å apart with intervening troughs of close-packed atoms 1.29 Å below the surface plane. The  $[1\bar{1}0]$  azimuth, which was the direction of the incident beam, is perpendicular to the ridge-trough structure and the  $[11\bar{1}]$  azimuth is parallel to it. The techniques of surface preparation and *in situ* cleaning, which are described elsewhere,<sup>4</sup> produce well-ordered surfaces with contamination levels less than 1% of the monolayer.<sup>12</sup> In addition, these surfaces all produced sharp diffraction of He (see Fig. 1 for the He scattering distributions from the surfaces actually used in this study), indicating further that they are clean, well ordered, and have a strong surface periodicity.

## RESULTS

In-plane scattering patterns at incident angles (measured from the surface normal) were obtained for room temperature (20 °C) Ar and Ne incident within the  $[1\bar{1}0]$  azimuth at temperatures of 900 °C, and 1100 °C, and 1300 °C (see Figs. 2-5). Neon scattering for beam temperatures of 20 °C, 230 °C, and 350 °C, and 45.5° incidence are shown in Fig. 6. All of the Ar patterns exhibit unilobular distributions whose peak maxima decrease with increasing angles of incidence and increase with surface temperature. Thus, the scattering lies

within what has been identified as the trapping dominated regime in agreement with the scattering from W(110).<sup>4</sup> A "trapped" atom is one which exchanges enough energy with the surface to become localized at the surface for a period of time which is long compared to lattice vibrations. Trapping dominated scattering distributions are those which result from a large fraction of the incident flux being initially trapped.

Neon scattering patterns obtained from the surface at 900 °C for different incidence angles are shown in Fig. 4. The pattern at 70° incidence has only a single broad maximum, but at the more normal angles (45.5°, 20°) the patterns exhibit the bilobular characteristics of surface rainbows, with some fine structure between the rainbow angles. The effect of increasing the surface temperature for an incidence angle of 45.5° is shown in Fig. 5. The rainbow peaks move toward the specular and decrease in intensity with the increasing surface temperature. The calculated first-order Bragg diffraction peaks for 20 °C Ne scattering from W(112) are indicated in Fig. 5 by arrows. Some of the fine

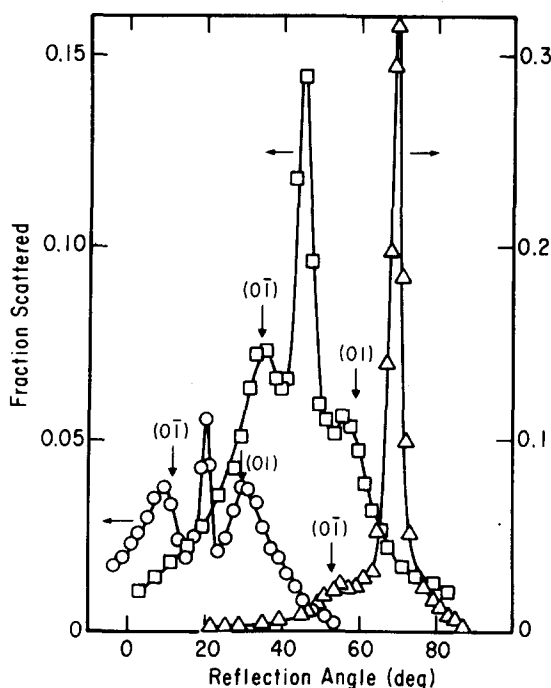


FIG. 1. Angular scattering distribution, 20 °C helium beam—900 °C W(112) at incidence angles: ○, 20°; □, 45.5°; △, 70°.

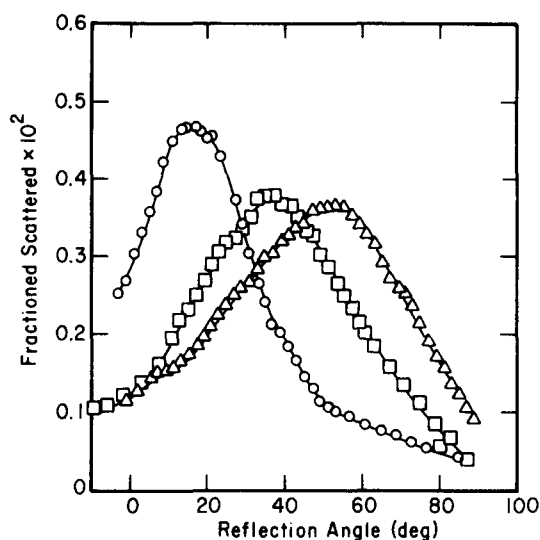


FIG. 2. Angular scattering distribution, 20 °C argon beam—900 °C at incidence angles: o, 20°; □, 45.5°; Δ, 70°.

structure appears to correlate with the position of the expected diffraction peaks.

In the Ne scattering patterns for different beam temperatures (Fig. 6), the intensity of the rainbow peaks increases and the position of the backscattered peak moves towards the specular angle, while the forward scattered peak position remains approximately constant as the beam temperatures increase. The fine structure between the rainbow peaks is altered with increasing beam temperature and in general cannot be indexed to recognizable diffraction features calculated for the increased beam temperature. The presence or absence of maxima in all these scattering patterns (Figs. 2–6) is reproducible even for different preparations of the surface. The absolute values of the intensity maxima are not reproducible to better than  $\pm 20\%$  for different surface preparations.

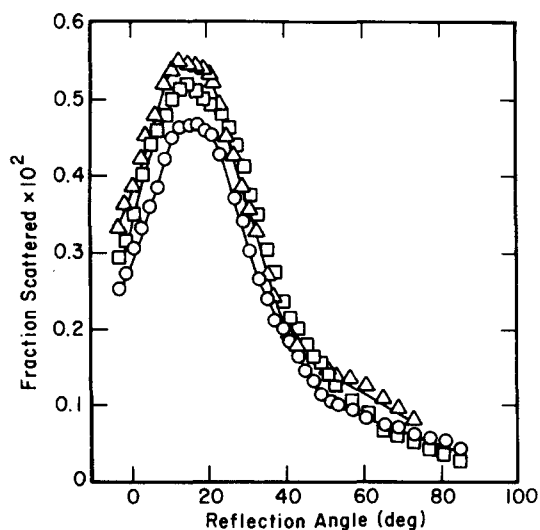


FIG. 3. Angular scattering distribution, 20 °C argon beam at 20° incidence on W(112) and surface temperatures: o, 900 °C; □, 1100 °C; Δ, 1300 °C.

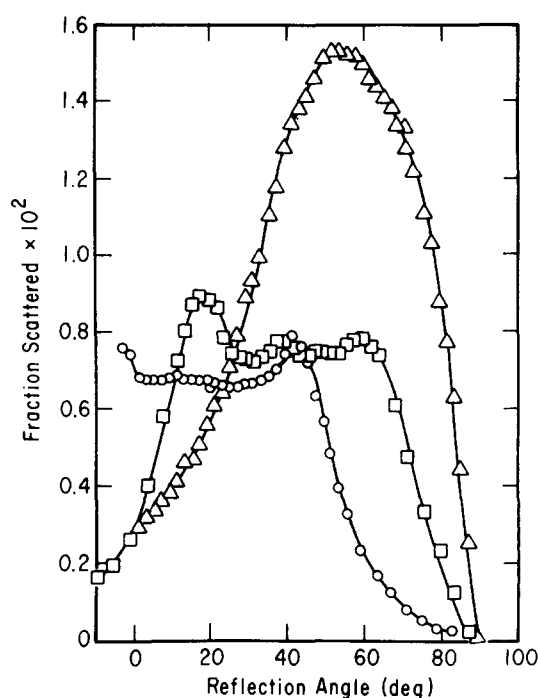


FIG. 4. Angular scattering distribution, 20 °C Ne beam—900 °C W(112) at incidence angles: o, 20°; □, 45.5°; Δ, 70°.

## DISCUSSION

The Ar scattering data obtained in this study for W(112) may be compared with that reported previously for Ar from W(110). The angular half-width obtained in this study for 20 °C Ar scattering from 900 °C W(112) at 45.5° incidence angle was 52°. Weinberg and Merrill<sup>4</sup> reported scattering patterns for 20 °C Ar from W(110) at relatively low crystal temperatures (100–500 °C). At 45° incidence angle, their angular half-width for the 300 °C surface temperature was 51°. Yamamoto and Stickney<sup>3</sup> reported Ar scattering from

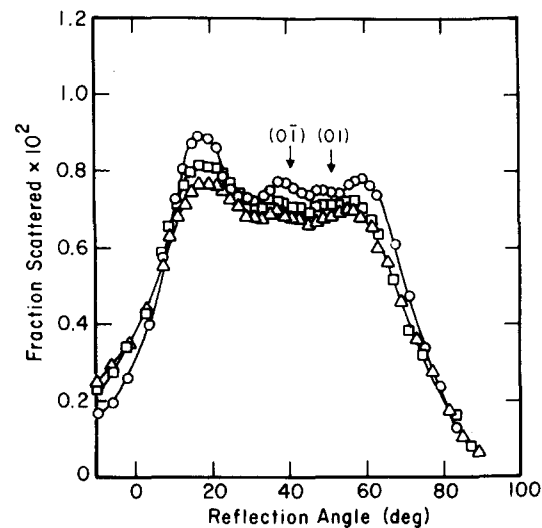


FIG. 5. Angular scattering distribution, 20 °C Ne beam at 45.5° incidence on W(112) at temperatures: o, 900 °C; □, 1100 °C; Δ, 1300 °C.

a low energy ( $\sim 275^\circ\text{C}$ ) nozzle beam scattering off a W(110) at a relatively high surface temperature of  $1830^\circ\text{C}$ . They reported angular half-widths of  $53^\circ \pm 3^\circ$  and  $54^\circ \pm 2^\circ$  for Ar scattering patterns at incident angles of  $40^\circ$  and  $50^\circ$ , respectively. Also, the shift of the Ar peak maximum ( $10^\circ$ ) for these results is about the same as that reported for the W(110) surface.<sup>3,4</sup> Thus, the interaction of Ar with both W(112) and W(110) is very similar.

The surface rainbows observed for the Ne scattering are similar to those reported for Ne on LiF by Smith *et al.*<sup>8</sup> In both cases the peaks approach one another as the incidence angle is increased, but in the LiF work both rainbow angles were clearly defined even at the most grazing angles investigated. In this work the two peaks coalesce at an incident angle of  $70^\circ$ .

Elastic semiclassical trajectory calculations<sup>13</sup> illustrate that the separation between the rainbow angles becomes greater as the amplitude of the surface periodicity is increased. The coalescence of the two rainbow peaks at grazing incidence angles manifests a decrease in the effective amplitude of the surface periodicity, presumably because of angular shadowing. The fact that the Ne rainbows do not coalesce with LiF, but Ar rainbows do,<sup>8</sup> indicates a stronger periodicity for the LiF surface than the W(112), where no surface rainbows are observed for Ar at any angles of incidence.

The variation of the Ne scattering patterns for a surface temperature at  $45.5^\circ$  incidence angle, shown in Fig. 5, demonstrates attenuation of the intensity of the scattered beam and movement of the rainbow peaks toward the specular with increasing surface temperature, which is in qualitative agreement with the experimental results of Smith *et al.*<sup>8</sup> for rainbow scattering from LiF and the calculations of McClure.<sup>14</sup> In Fig. 6 the position of the backscattered peak, the peak nearest the surface normal, moves toward the specular angle as the beam temperatures increase also in qualitative agreement with the results of Smith *et al.*<sup>8</sup> and the calculations of McClure.<sup>14</sup> According to the phenomenological classification previously suggested,<sup>2,4</sup> Ne scattering from tungsten surfaces should be in the inelastic scattering regime but clearly not dominated by trapping. Comparisons of the elastic semiclassical trajectory calculations with these results<sup>13</sup> show that this is indeed the case, i.e., large intensities are backscattered outside the elastic rainbow angle, indicating strong inelastic interactions for this system. On the other hand, Ar scattering would be expected to be in the trapping dominated regime,<sup>4</sup> and indeed the patterns in Fig. 3 show the characteristic increase in peak intensity at the peak maximum with increasing surface temperature and a slight but recognizable shift towards normal angles.

Though no Ne or Ar scattering has as yet been measured for  $[11\bar{1}]$  azimuthal direction, the scattering of helium in that direction<sup>10,12</sup> indicates that the surface periodicity is indeed significantly less than in the  $[1\bar{1}0]$  azimuth, as would be expected from the surface crystallography. No rainbow scattering would be expected in the  $[11\bar{1}]$  azimuth.

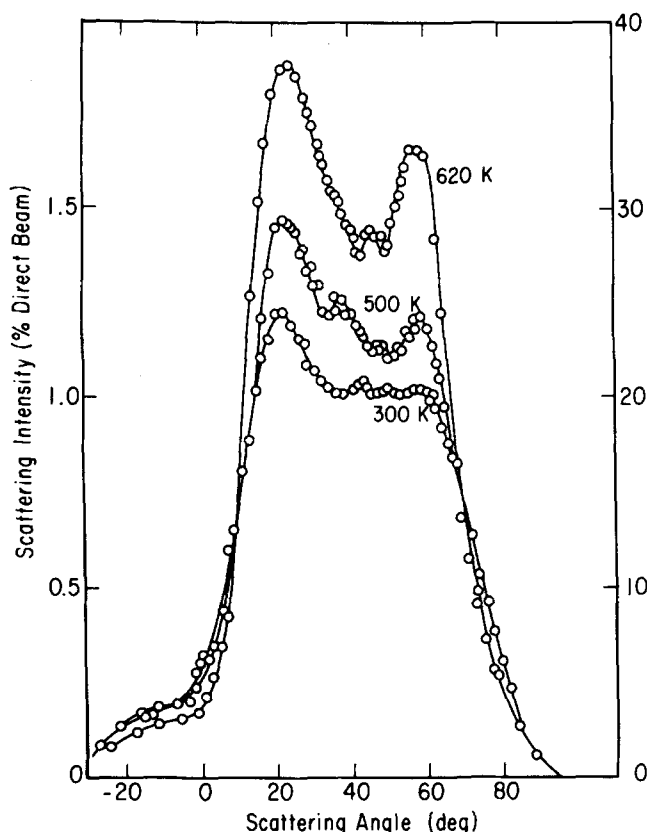


FIG. 6. Angular scattering distribution, Ne on W(112) at a temperature of  $900^\circ\text{C}$ , incidence angle of  $45^\circ$ , and beam temperatures,  $\circ$ ,  $20^\circ\text{C}$ ;  $\square$ ,  $230^\circ\text{C}$ ;  $\triangle$ ,  $350^\circ\text{C}$ .

## CONCLUSIONS

Clean W(112) surfaces scatter Ar in a manner very similar to its scattering from W(110) surfaces, i.e., unilobular patterns in the trapping dominated regime. The scattering of Ne, however, exhibits strong rainbowlike features, but there are indications that the interactions are highly inelastic. The effect of angle of incidence, surface temperature, and gas temperature are qualitatively similar to that found for Ne scattering from LiF surfaces, which exhibit rainbow patterns also. These features are predicted qualitatively by the classical calculations of McClure<sup>14</sup> and also the semiclassical trajectory calculations.<sup>13</sup> The semiclassical calculations, however, do not predict the quantitative details because to date they have included only elastic trajectories. Though no measurements of Ne scattering along the smooth direction of W(112) have been made, by analogy with the coalescence of the rainbow peaks into a unilobular pattern at  $70^\circ$  incidence one expects no rainbow scattering in the  $[11\bar{1}]$  azimuth.

## ACKNOWLEDGMENTS

This work was supported by AFOSR Grant No. 72-2218. R. E. W. acknowledges the financial support of Tau Beta Pi as a Spencer Fellow. J. J. E. acknowledges support as a NATO Postdoctoral Fellow.

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