scaling hypothesis used by McMillan and by Hopfield in their work on the theory of strong-coupling superconductors is questionable. Further theoretical work is required to convert these measurements into the McMillan parameter for the host atoms.

We would like to acknowledge several useful discussions with Dr. M. Thorpe and Dr. W. Visscher.

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*Work performed under the auspices of the U. S. Atomic Energy Commission.

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Atomic and Molecular Diffraction of Helium and Deuterium from a Tungsten Carbide Surface Characterized by Low-Energy Electron Diffraction*

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(Received 28 August 1970)

The diffraction of thermal beams of helium and deuterium has been observed from a carbide overlayer on tungsten (110). The diffraction grating derived from the atomic and molecular diffraction agrees with that determined by electron diffraction. Peaks through second order have been resolved and helium peaks are characterized by extremely high intensities and narrow half-widths. Use of atomic diffraction to study species which adsorb in a regular array is suggested.

After the de Broglie postulate of the wave nature of matter in 1924, there were numerous attempts to observe the phenomenon experimentally via diffraction from a two-dimensional surface grating. In 1927 Davisson and Germer observed the diffraction of low-energy electrons which had been scattered from a single crystal of nickel.[1] In the early 1930's, Stern and co-workers observed the atomic and molecular diffraction of helium and hydrogen thermal beams from LiF and NaCl single crystals.[2-5] At the same time, Johnson observed the diffraction of a thermal beam of hydrogen atoms from LiF.[6] During the past forty years there have been many investigations of atomic and molecular diffraction from LiF in particular.[7-13] These workers have investigated the gas-surface interaction in both elastic-and inelastic-scattering events. Also there have been numerous attempts to observe atomic diffraction from other surfaces, notably metal surfaces (for a discussion see, e.g., Palmer, Saltsburg, and Smith[14] and Stoll and Merrill[15]) but none has been found except for the alkali halides, NaCl and LiF. In this Letter we report the diffraction of thermal He and D_2 beams from a W(110) surface with an overlayer carbide structure in a periodic (3×5) array rotated 35° with respect to the W substrate. The $R(3\times5)$ 35° was confirmed by low-energy electron diffraction (LEED). This carbide structure is similar to one previously reported on W(110) by Stern.[16]

The experimental apparatus has been described in detail previously[17]; very briefly it consists of a thermal molecular beam generated by an effusive source together with a LEED assembly in an ultrahigh-vacuum chamber (background pressure less than 7×10^{-11} Torr). Detection of either the direct beam or the scattered beam in the principal scattering plane is accomplished in the dc mode using a rotating probe connected to a stationary mass spectrometer. The angular resolution of the probe is approximately 2°. The detected signal is proportional to the scattered gas flux. With the beam in operation, the background pressure remains below $(3\text{-}4)\times10^{-10}$ Torr. Prior to measuring a scattering distribution the crystal was flashed to remove adsorbable background gases which were mainly H_2, CO, and CO_2. The W surface was spark cut from a 99.999%-W single crystal after having been oriented to within $\frac{1}{4}°$ of the (110) surface, polished, and finally chemically etched just prior to insertion into the ultrahigh-vacuum chamber.

The $R(3\times5)$ 35° carbide surface was visible in the LEED prior to any in situ treatment, and it was stable at an annealing temperature of 1800°K. That the overlayer was carbon was inferred from the previous LEED results of Stern[16] and was later confirmed when it was removed by heating in either O_2 or H_2. In the former case CO and CO_2 mass spectrometer peaks increased in intensity during the chemical cleaning, and in the latter case the usual hydrocarbon peaks increased.

The diffraction grating in the principal scattering plane was determined to be about 10° off the fifth-order spacing in the $R(3\times5)$ pattern. Thus the diffraction grating is $d=5\times2.23\times\cos10°$ $=11.0$ Å. All gas temperatures were 295°K, and the corresponding wavelength of both the He and the D_2 beams is thus 0.588 Å.[18] The expected diffraction angles through second order are indicated by arrows in Figs. 1-3. The experimental arrangement precluded varying the azimuthal angle, so it was impossible to maximize all diffraction peaks simultaneously in the principal scattering plane. However, by tilting the crystal each peak could be approximately maximized separately.

Figure 1 shows a He-scattering pattern for an incidence angle θ_i of 45° and a surface temperature T_s of 375°K (solid line). The (00), (10), and (20) diffraction peaks are all evident. None of the peaks are individually maximized, but the peaks are very intense nevertheless. Specular maxima which are 57% of the incident direct beam have been observed for a He beam with $\theta_i=45°$ and T_s $=375°$K. This may be compared with the most intense reflected beam previously reported—He scattered from a Pt(111) surface with $\theta_i=45°$, $T_s=375°$K, and $T_{\mathrm{He}}=1000°$K, which had a specular maximum of approximately 25% of the direct beam.[15] The He did not diffract from the clean Pt(111) surface. Also plotted in Fig. 1 (dashed line) is a helium scattering distribution from a clean W(110) surface. Like the Pt(111) scattering it is broader and less intense and exhibits no diffraction. The extreme narrowness of the individual diffraction peaks in Fig. 1 should also be noted. For example, the specular (00) peak half-width is only about 3.5° which may be compared with an incident (direct-beam) half-width of about 7.5°. This remarkable coherence is even more unusual in view of the fact that the incident beam has the usual thermal spread in wavelength.

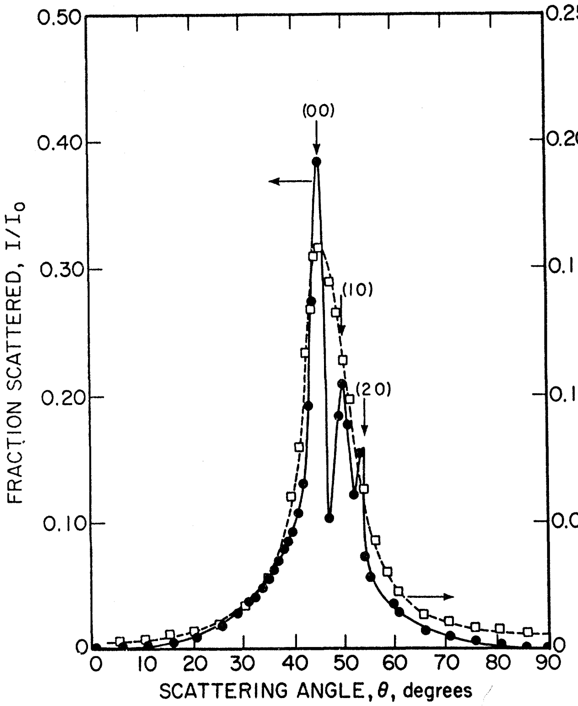

FIG. 1. Helium scattering from a W(110) surface. Circles, helium diffraction pattern from $R(3\times5)$ carbide surface; $T_s=375°$K, $T_g=375°$K, $\theta_i=45°$. Squares, helium scattering from clean surface; $T_s=375°$K, T_g $=375°$K, $\theta_i=45°$.

Figure 2 shows a He-scattering pattern for an incident angle of 20° and a surface temperature of 375°K with the (00) and $(\bar{2}0)$ diffraction peaks evident and a He-scattering pattern for a 66° incident angle and a surface temperature of 375°K, which exhibits the (00) and $(\bar{1}0)$ diffraction peaks.

The results for D_2 scattering at an incidence angle of 45° and a surface temperature of 625°K are shown in Fig. 3. The (00), (10), and (20) diffraction peaks are resolved although less completely than in the case of He.[19] Diffraction of D_2 from LiF is also less intense and less well resolved than that for He.[11-13] The reason for this is that a larger fraction of the D_2 is trapped in its (deeper) potential well with the surface,[20] and there can be rotational-phonon coupling between the D_2 and the solid.[21] The D_2 cannot be scattered from the clean tungsten carbide surface at a surface temperature below approximately 625°K

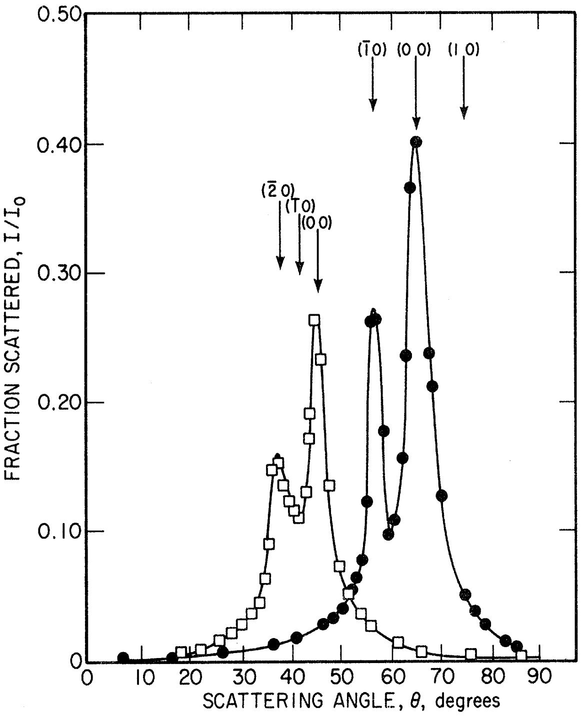

FIG. 2. Helium diffraction from a W(110) $R(3\times5)$ carbide surface. Circles: $T_s=375°\text{K}$, $T_g=375°\text{K}$, $\theta_i=66°$. Squares: $T_s=375°\text{K}$, $T_g=375°\text{K}$, $\theta_i=20°$.

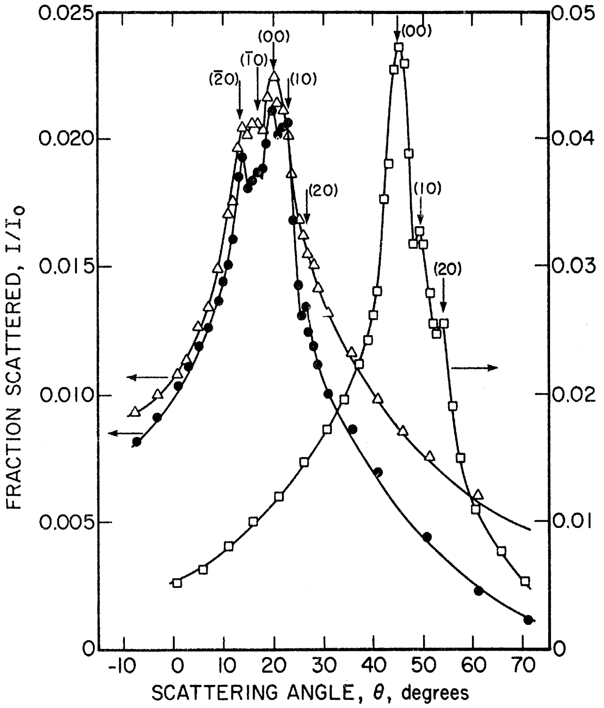

FIG. 3. Deuterium diffraction from a W(110) $R(3\times5)$ carbide surface. Circles: $T_s=625°\text{K}$, $T_g=375°\text{K}$, $\theta_i=20°$. Triangles: $T_s=775°\text{K}$, $T_g=375°\text{K}$, $\theta_i=20°$. Squares: $T_s=625°\text{K}$, $T_g=375°\text{K}$, $\theta_i=45°$.

since the D_2 adsorbs on the surface and is only completely desorbed at about that temperature.

The results for D_2 scattering at an incident angle of 20° and surface temperatures of 625 and 775°K are also shown in Fig. 3. For $T_s=625°\text{K}$, the $(\bar{2}0)$, $(\bar{1}0)$, (00), (10), and (20) diffraction peaks are all partially resolved, while for the 775°K surface the (00), $(\bar{1}0)$, and $(\bar{2}0)$ peaks are resolved. It should be emphasized again that no single peak is at its maximum, and since the incident beams are of the same intensity, it is clear that the 625°K surface peaks are further removed from their individual maxima than are the 775°K peaks. At its maximum, the 625°K (00) peak is more intense than that of the 775°K one because of thermal roughening of the surface at the higher surface temperature.

The results presented here are noteworthy for a number of reasons. First, it is of interest that after so many years atomic and molecular diffraction has been observed, finally, from a surface other than an alkali halide. More important, however, may be the possibility of analyzing surface structures resulting from adsorption by atomic scattering as an alternative to (or in addition to) LEED and high-energy electron diffraction (HEED). In electron diffraction the diffracted particles penetrate into the solid even at the lowest voltages and/or angles of incidence, so the analysis of surface structures via intensity data is always complicated by bulk effects and the interaction of the sorbate diffraction with the substrate diffraction. Multiple-scattering effects, strong inelastic interactions of diffracted electrons, uncertainties about the inner potential (electron self-energy), and unknown phase shifts at the scattering centers also complicate the intensity analysis, as is well known. In atomic scattering, on the other hand, only the surface is probed (on metals apparently only the sorbate) so the analysis of intensity data from atomic diffraction should be considerably more definitive. The utility of this method in analyzing surface structures depends on the ability to resolve diffraction peaks from the diffuse scattering background. For example, when C_2H_4 is adsorbed on Pt(111) in a regular (2×2) array according to LEED, the specular peak intensity of the He beam is so diminished that any diffraction peaks which might be present are completely obscured.[17] Perhaps velocity selection of the scattered beam can be made to effect the separation. Even without velocity selection, however, it is expected that there are a number of gases which adsorb in a regular array and which will show atomic diffraction that can potentially be analyzed for definitive structure determination. This should be applicable for insulator and semiconductor surfaces in addition to metal surfaces, and the difficulty of surface charging which is present with electron diffraction is obviated with diffraction of neutrals. As an example, when H_2 adsorbs atomically in a (1×1) array on the tungsten carbide surface, the zero-, first-, and second-order diffraction peaks, though somewhat attenuated, can still be resolved. Such experiments designed to explore the range of adsorbates which exhibit He diffraction are continuing in this laboratory.

A more complete presentation of the diffraction of He and D_2 from the $R(3\times5)$ tungsten carbide, as well as Ne and Ar scattering from that surface, and He and D_2 scattering from a (1×1) tungsten carbide surface will be presented in a future publication.

One of us (W.H.W.) acknowledges the support of a National Defense Education Act pre-doctoral fellowship.

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*Work supported by U. S. Air Force Office of Scientific Research Grant No. 68-1409.

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[19] The specular maximum of D_2 at $\theta_i = 45°$, $T_s = 625$°K is about 5%, while the specular maximum of He under the same conditions is about 50% of the incident-beam intensity for this tungsten carbide surface.

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Experimental Verification of First-Order Rotational Effects in the Magnetoelastic Properties of an Antiferromagnet*

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(Received 27 August 1970)

The experimental magnetoelastic properties of antiferromagnetic MnF_2 are found in certain specific instances to be completely inconsistent with the usual small-strain magnetoelastic theory. Rigorous application of finite-deformation magnetoelastic theory including the effect of the rotational component of the shear deformation leads to results which are in excellent agreement with experiment.

The purpose of this paper is to provide experimental verification of finite-deformation magnetoelastic theory when applied to an antiferromagnetic, elastic medium. It will be shown that the neglect of the rotational component of an elastic shear deformation by the usual small-strain magnetoelastic theory[1,2] leads to first-order results both qualitatively and quantitatively inconsistent with experiment. This is the first experimental demonstration of the validity of finite-deformation theory for an antiferromagnet. Eastman[3] has shown that magnetoelastic effects in yttrium iron