Apart from these difficulties the present results demonstrate that UPS data from adsorbed Xe atoms provide a sensitive tool for probing local surface inhomogeneities. In particular, it is suggested that this technique can be used in selective adsorption studies to identify surface compositions of multicomponent systems. The weakness of the xenon-metal bond and the low temperature to be applied guarantee that no adsorption-induced segregation will occur. As demonstrated in the case of the Ir(100) surface which reconstructs only in the topmost atom layer,[17] the xenon adsorption method should also give the surface composition of the outermost atomic layer only.

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Temperature Dependence of the Shear Modulus and Melting of the Two-Dimensional Electron Solid

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The temperature dependence of the shear modulus μ in the two-dimensional electron solid has been determined in a computer simulation. It is found that at low temperatures T, μ decreases linearly with increasing T. A sharp drop of μ together with the onset of electron diffusion in the range $140>\Gamma>120$, where $\Gamma = e^2(\pi n_s)^{1/2}/k_B T$, suggestes a melting point consistent with the experiment by Grimes and Adams. The results presented here are consistent with recent theories of dislocation-mediated melting in two dimensions.

In a recent experiment, Grimes and Adams[1] have observed the formation of a two-dimensional (2D) electron solid for electrons on the surface of liquid helium. They find a melting temperature T_m which we write as $\Gamma_m \simeq 137 \pm 15$, where $\Gamma = (\pi n_s)^{1/2} e^2/k_B T$ and n_s is the areal electron density.

A theoretical estimate for the melting point of this system has first been given by Platzman and Fukuyama.[2] They use a self-consistent phonon theory to calculate the effects of phonon-phonon interactions and find an instability in the transverse mode at $\Gamma = 2.8$ which they identify with the melting point.

More recently, an estimate for Γ_m has been given by Thouless,[3] based on the theory of dislocation-mediated melting, which was proposed by Kosterlitz and Thouless,[4] and analyzed in greater

detail by Halperin and Nelson[5] and by Young.[6] This theory predicts a universal relation between the melting temperature T_m and the T-dependent Lamé elastic constants λ and μ,

$$\mu(\mu+\lambda)/(2\mu+\lambda) = 4\pi k_B T_m/b_0^2. \quad (1)$$

Here, b_0 denotes the lattice constant. Using the $T=0$ values,[7] $\lambda=\infty$ and $\mu = 0.245\,065 e^2 n_s^{3/2}$, Thouless obtains a value $\Gamma_m = 78.71$.

In view of the large difference between this theoretical estimate and the experimental result, one may question the applicability of this theory. In fact, the shear modulus would have to *decrease* by 40% from its $T=0$ value if Eq. (1) is to hold for a melting point $\Gamma_m \approx 140$. The calculation by Platzman and Fukuyama[2] suggested, however, that μ should *increase* with temperature over the range of interest.

So far, two numerical simulations of the 2D electron solid have been reported: (i) a "molecular dynamics" (MD) simulation by Hockney and Brown[8] who reported a lambdalike behavior of the specific heat at $\Gamma \approx 95 \pm 2$ which they identified as the melting point; (ii) a Monte Carlo calculation by Gann, Chakravarty, and Chester,[9] who find a melting point $\Gamma_m \approx 125 \pm 15$, consistent with the experiment by Grimes and Adams.[1] None of these works has addressed the question if the theory of dislocation-mediated melting is applicable to the 2D electron solid. In particular, the behavior of the elastic constants about which this theory makes the powerful prediction of Eq. (1) has not been investigated.

In this work I study the temperature dependence of μ via a MD simulation in the solid phase. My principal result is that there is a significant reduction of μ, linear in T for temperatures from $T=0$ until slightly below T_m, which we attribute to phonon-phonon interactions. It is then possible with use of the renormalization-group equations of Halperin and Nelson,[5] with a plausible choice for the dislocation core free energy, to obtain the additional reduction of the elastic constants near T_m, due to the polarizability of dislocation pairs, which enables Eq. (1) to be valid at T_m. In my MD simulation I observe a sharp drop in the shear-wave frequency together with the onset of particle diffusion in the interval $140 > \Gamma > 120$ which suggests a melting point in this range, consistent with both Grimes and Adams[1] as well as Gann, Chakravarty, and Chester.[9]

My MD calculation is done on a system with 780 ($=26\times 30$) electrons in a uniform positive background and subject to periodic boundary conditions. The forces are calculated by the method described by Fisher, Halperin, and Morf.[10] It is similar to the one employed by Hockney and Brown[8]: The summation over interactions between particles with separation less than a radius R_c is carried out exactly while the contribution from particles with larger separations is calculated by means of a mesh method using fast Fourier transforms. For the present calculation we use $R_c = 4.1 b_0$ and a mesh with 64×64 points, which assures that the small errors in the calculated forces are incommensurate[5] (to the extent possible in a finite system) with the lattice containing 26×30 particles.

For the dynamic simulation we use a canonical precedure[11] in which each particle is coupled to a heat bath. The equations of motion for particle i at position $\vec{r}_i$ are

$$m\ddot{\vec{r}}_i = \vec{F}_i + \vec{\varphi}_i(t) - m\gamma\dot{\vec{r}}_i, \quad (2)$$

where $\vec{F}_i$ is the Coulomb force and $\vec{\varphi}_i = (\varphi_i^{(1)}, \varphi_i^{(2)})$ is a Gaussian white-noise force representing the heat bath at temperature T and obeys the conditions $\langle\vec{\varphi}_i\rangle = 0$ and $\langle\varphi_i^{(k)}(t)\varphi_j^{(l)}(t^1)\rangle = 2m\gamma k_B T \times \delta(t-t^1)\delta_{ij}\delta_{kl}$. The coupling to the heat bath is controlled by the parameter γ.

The numerical integration of Eq. (2) is done by means of the finite-difference method of Ref. 11 with a time step $\Delta = 2\pi/21.46\omega_0$, where[2,7] $\omega_0^2 = 8e^2/mb_0^3$. This time step corresponds to 1/18 of the period of the fastest longitudinal mode at $T=0$, which guarantees sufficient numerical accuracy.

For small wave numbers q the transverse phonon frequency $\omega_t(q)$ is related to the shear modulus by $\omega_t^2(q) = \mu q^2/mn_s$. This allows a dynamical determination of μ by analysis of the time dependence of the transverse modes $x_q(t)$. In equilibrium these modes will obey a Langevin equation of a harmonic oscillator,

$$\ddot{x}_q(t) + \omega_q^2 x_q(t) + \beta_q \dot{x}_q(t) = \varphi(t), \quad (3)$$

where $\varphi(t)$ is a stochastic force with the usual properties (see above).

Assuming the validity of Eq. (3) with unknown parameters ω_q and β_q one can define the probability $P(x,t|x_0,\dot{x}_0)$ of observing a value x at time t provided that one knows the values $x_q(t_0)=x_0$ and $\dot{x}_q(t_0)=\dot{x}_0$ at time t_0. This probability depends parametrically on ω_q and β_q. According to Chandrasekhar[12] it is a Gaussian centered at $x = x_0 a(t) + \dot{x}_0 b(t)$, with variance

$$\sigma^2 = \langle x_q^2\rangle[1 - \exp(-\beta_q t) - \beta_q a(t) b(t)],$$

where

$$a(t) = \exp(-\beta_q t/2)[\cos\omega_1 t + \sin(\omega_1 t)\beta_q/2\omega_1]$$

and

$$b(t) = \omega_1^{-1} \exp(-\beta_q t/2) \sin\omega_1 t,$$

with $\omega_1 = (\omega_q^2 - \beta_q^2/4)^{1/2}$. From the observed values $x_q(t_i)$, $\dot{x}_q(t_i)$ $(i = 1, \ldots, M)$ I form the logarithm of the likelihood function

$$\mathcal{L}(\omega_q, \beta_q) = \sum_k^M \sum_{i>k}^M \ln P(x_q(t_i), t_i | x_q(t_k), \dot{x}_q(t_k)), \quad (4)$$

and determine ω_q and β_q by maximizing $\mathcal{L}(\omega_q, \beta_q)$. The summation over k is arbitrarily done in steps of 250. In contrast to conventional methods for determining ω_q which make use of the Fourier transforms of correlation functions, this method works well even if only few periods of the mode are observed and in cases where the damping β_q is considerable. In addition, it is amenable to a χ^2 test.

The simulation is started at $T = 0$ with a perfect hexagonal crystal. To change temperature the system is coupled to a heat bath at the desired temperature during 2500 time steps, with a coupling $\gamma = (500\Delta)^{-1}$. During subsequent 2500 time steps, γ is set equal to zero and in that period the shear modulus is determined. The temperature is calculated from the mean kinetic energy.

The results of my simulation are shown in Fig. 1. The circles represent the ratio $R = \mu(\Gamma)/\mu(\Gamma = \infty)$ as a function of Γ^{-1}. The full circles represent values obtained in heating the system up; the open ones are obtained in cooling down after the system has been heated to a value $\Gamma = 120$. At low temperatures ($\Gamma \to \infty$), one observes a linear decrease of R amounting to approximately 15% at $\Gamma = 200$.

For $140 > \Gamma > 120$ we observe a strong decrease of μ. Pictures of the system show that in this Γ range bound dislocation pairs appear in increasing number, and below $\Gamma \sim 118$–120 a network of grain boundaries and/or dislocations is formed. Also displayed, in the inset in Fig. 1, are results concerning particle diffusion. The crosses represent the fraction of particles moving further than one lattice constant in 1000 time steps during the sequence $\Gamma = (122, 127, 129, 129, 136)$, corresponding to cooling down. One can observe a strong rise in the particle diffusion rate in the same Γ range where the shear modulus shows its significant decrease. This suggests a melting point in the range $120 < \Gamma_m < 140$, in qualitative agreement with the experimental result by Grimes and Adams[1] and with the Monte Carlo result by Gann, Chakravarty, and Chester.[9]

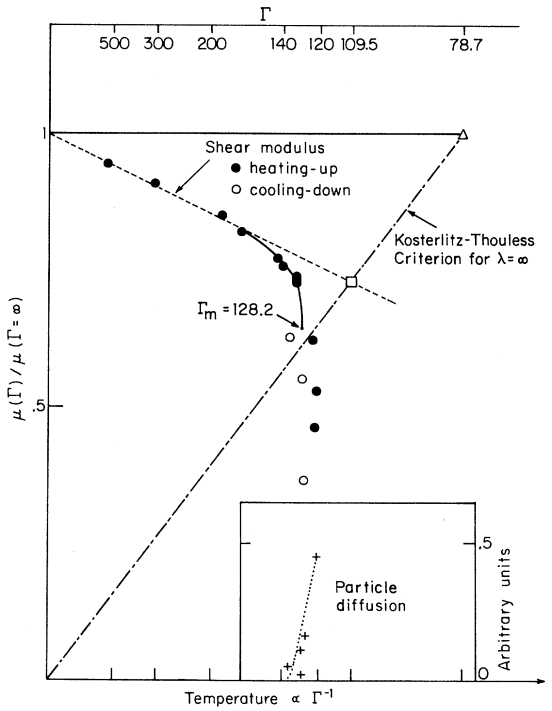

FIG. 1. Temperature dependence of shear modulus μ and particle diffusion. The circles represent the MD results for $\mu(\Gamma)/\mu(\Gamma = \infty)$ as function of Γ^{-1}. The observed particle diffusion is shown in the inset (dotted line and plusses). The full line, ending at $\Gamma_m = 128.2$, displays the RG results with use of a linear extrapolation for the shear modulus (dashed line) as Γ-dependent bare values. The Thouless value $\Gamma = 78.7$ (triangle) is obtained with use of $T = 0$ elastic constants.

Before proceeding to a comparison with the Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory of melting I would like to discuss a serious problem in this simulation. While in the defect-free solid phase the equilibration time is determined by the damping of the slowest phonon modes and can be cut down by coupling the system to a heat bath, however, as the melting point is approached, it is determined by much slower processes like defect generation and defect diffusion. As a consequence, all results become less reliable, which is illustrated by the difference in the shear modulus observed in heating up (full circles) and cooling down (open circles). Which of these results is closer to the equilibrium values can only be answered reliably by observing the system during much longer periods. It also turned out to be impossible (within 15 000 time steps) to get back to a defect-free

system once the system is heated below a value $\Gamma \sim 118$, where a network of grain boundaries and/or dislocations appears. In view of this, it is not surprising that Hockney and Brown[8] obtained results different from mine. They started with particles at random positions and the time the allowed for the system to reach equilibrium is short even compared to phonon relaxation times. Their results are therefore likely to be affected by nonequilibrium effects. This has been discussed by Gann, Chakravarty, and Chester,[9] who found no anomaly in the free energy for $\Gamma \sim 95$.

Let us now compare the observed decrease of μ below $\Gamma \sim 150$ with the one expected from the KTHNY theory of melting. We do this by integrating the renormalization-group (RG) equations, derived by Halperin and Nelson,[5] with appropriate initial values for the elastic constants $\mu(l=0)$, $\lambda(l=0)$, and for the fugacity $y(l=0)$. For the definition of the initial values $\lambda(l=0)$ and $\mu(l=0)$ I make the following assumptions: (i) $\lambda(l=0)=\infty$, i.e., in the absence of dislocations the lattice remains incompressible. (ii) Since bound dislocation pairs (like other defects,[10] e.g., vacancies and interstitials, but unlike phonons) have a finite excitation energy[10] their effects on the elastic constants will decrease exponentially at low temperatures. It is therefore natural to assume that the linear decrease of $\mu(T)$ at low T is due only to phonon interactions and as a simple approximation which requires no adjustable parameters, one may use a linear extrapolation $\mu_L(\Gamma)=\mu(\Gamma=\infty)(1-30.8\Gamma^{-1})$ (dashed line in Fig. 1) as a Γ-dependent "bare" (with respect to dislocations) shear modulus $\mu(l=0)$.

The initial value $k_B T \ln y(0)$ is determined by the core energy E_c of a dislocation, which has been calculated at $T=0$ by Fisher, Halperin, and Morf.[10] With the lattice constant as length unit, the core energy $\bar{E}_c$ has the value $\bar{E}_c=(0.1\pm 0.02)\times n_s^{1/2}e^2=\bar{C}\mu b_0^2/2\pi$, with $\bar{C}=2.2\pm 0.4$. Since in the definition of E_c in Ref. 5 an unspecified core diameter a is used as a length unit, the appropriate core energy E_c becomes a dependent: $E_c=(\mu b_0^2/2\pi)(\bar{C}+\ln a/b_0)$. In addition, taking into account the number of possible sites N for a dislocation in an area a^2, $N=a^2/(\frac{3}{4})^{1/2}b_0^2$, which has been set equal to 1 in Ref. 3, we obtain $y(0)=(\frac{4}{3})^{1/2}(a/b_0)^{2-\tilde{K}}e^{-\tilde{K}\bar{C}}$, where $\tilde{K}=\mu(l=0)b_0^2/(2\pi k_B T)$. Assuming that the core energy E_c is renormalized by phonon-phonon interactions in the same proportion as the shear modulus, I take $\tilde{C}$ to be temperature independent.

The solid curve in Fig. 1 shows the result of the RG calculation with the starting length scale $a=2b_0$ and with the zero-temperature value 2.2 for the parameter $\tilde{C}$. The melting point is at $\Gamma_m=128.2$. The agreement between the MD calculation and the KTHNY theory looks satisfactory.

It is interesting to note that because of the effects of dislocations, the Lamé coefficient λ gets renormalized to a finite value at the melting point, $\lambda(\Gamma_m)/\mu(\Gamma_m)\sim 23$. This explains why the shear modulus exhibits a discontinuity which is slightly ($\sim 4\%$) larger than the one obtained from the Kosterlitz-Thouless criterion [Eq. (1)] for $\lambda=\infty$.

The sensitivity of the estimated melting point to the particular choice of the parameters a and $\bar{C}$ can be summarized as follows: For fixed $a=2b_0$, for values of $\bar{C}$ in the interval $1.8<\bar{C}<2.6$, the melting point varies in the range $142>\Gamma_m>120$, and for $\bar{C}\to\infty$ it tends to its lower limit $\Gamma_m=109.5$ (□ in Fig. 1). For fixed $\bar{C}=2.2$, for values of a between $b_0<a<4b_0$, melting occurs between $132>\Gamma_m>125$.

We may therefore conclude that my estimate for the melting point obtained from the dislocation theory of melting is consistent with both the experimental results of Grimes and Adams[1] as well as the numerical results by Gann, Chakravarty, and Chester[9] and those of the present work.

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Evidence for a Clean $(\sqrt{2}\times\sqrt{2})R45°$ Surface Structure on Cr(100)

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Low-energy electron diffraction observations of carefully cleaned and annealed Cr(100) surfaces show a sharp and intense $(\sqrt{2}\times\sqrt{2})R45°$ structure. Auger-electron spectroscopy measurements indicate that this "anomalous" structure is actually a clean-surface effect. A strong contamination-sensitive feature is revealed by angle-resolved photoemission and it is suggested that reconstruction results from an instability connected with a peak near E_F in the surface density of states of the Cr(100) (1×1) surface.

The simplest model of reconstruction considered for low-index faces of metals with respect to the bulk is just a relaxation in the direction normal to the surface. However, it was soon recognized that certain crystallographic orientations of Pt[1] and Au[2] show a more complicated surface reconstruction. More recently the existence of a surface phase transition near room temperature has been conclusively demonstrated for W(100) and Mo(100) surfaces.[3-5] Chromium has a body-centered-cubic lattice and 5*d* electrons and thus it is, in many respects, similar to Mo and W. Most likely interesting facts should be learned from investigations of chromium surfaces.

In this Letter we report on the successful preparation of the clean Cr(100) surface which we studied using Auger electron spectrometry (AES), low-energy electron diffraction (LEED), and photoemission. We find that this surface is not stable in the (1×1) configuration and that reconstruction into a $(\sqrt{2}\times\sqrt{2})R45°$ structure occurs. Basically, as to the corresponding electronic structure, it is found by ultraviolet photoemission (UPS) that a sharp feature in the energy distribution curves (EDC's) at ~1 eV below the Fermi level (E_F) is associated with the reconstructed surface and it is suggested that the reconstruction of the Cr(100) surface is an electronically driven lattice distortion due to a peak near E_F in the surface density of states of the undistorted (1×1) surface.[6,7]

Measurements were carried out in an ultra-high-vacuum electron spectrometer equipped with a windowless discharge lamp for UPS and a rotatable hemispherical energy analyzer collecting electrons ejected within a cone of 2° semiangle. An electron gun for AES and four-grid LEED optics were also available. After mechanical and electropolishing, the well-oriented single crystal was cleaned *in situ* by Ar-ion bombardment and annealing at various temperatures below 900 °C. Annealing above 600 °C led to impurity segregation of carbon and sulfur but cleaned the surface with respect to oxygen. Generally a $c(2\times2)$-S structure was then observed. We note here that this structure is very different from the $c(2\times2)$ structure of clean Cr(100) described below since no sulfur at all was detected for the latter and even a qualitative inspection of the LEED spectra showed a striking difference in the beam intensity versus energy curves. Actually in the final stage of the cleaning procedure the annealing temperature was kept below 500 °C. Only carbon and oxygen were then still detected by AES and a sharp and intense $(\sqrt{2}\times\sqrt{2})R45°$ LEED pattern was observed. We have carefully estimated the residual amounts of carbon and oxygen using AES. The results are summarized in Table I for four typical