Size Dependence of the Shear Modulus in a Two-Dimensional Solid

Toxvaerd[1] measured the shear moduli of 64-, 256-, and 1024-particle triangular-lattice crystals in two dimensions, using a (nearest-neighbor) "Weeks-Chandler-Andersen" truncated Lennard-Jones potential. The moduli were determined by application of small shear strains, 0.005 or 0.010, and measurement of the time-averaged shear stress, with use of molecular dynamics. The moduli fell on a straight line when plotted versus $\ln N$, within the (3–10)% statistical uncertainty of the results. Plots of the same data versus $1/N$ are described less well by a straight line. Toxvaerd therefore suggested that the shear modulus varies logarithmically with system size. Such a variation would have the bizarre consequence that the *shear modulus would vanish for sufficiently large crystals* (around 10^{11} particles, on the basis of Toxvaerd's straight line).

Because we saw no physical reason why two-dimensional moduli should vanish in the solid phase, we undertook a series of calculations to elucidate the number dependence of the two-dimensional shear modulus. For this purpose quasiharmonic lattice dynamics proved to be a useful tool. Exact results were generated for a wide range of system sizes.

We used two different and independent methods for determining moduli: (1) a direct determination of the pressure tensor for a standard crystal, using the quasiharmonic pair distribution function; (2) a finite-difference calculation of the second derivative of the Helmholtz free energy (using strains of -0.001, 0.000, and $+0.001$). In this way we determined moduli[2] for crystals of from 16 to 160 000 particles. Results at three different densities, two of those studied by Toxvaerd as well as the zero-temperature, zero-pressure number density, $\rho \equiv (Ns^2/V) = (4/3)^{0.5}$, had nearly identical number dependence. Fitting the data to the functional form

$$G(T,N) = G(0,\infty) + \left[\frac{kT}{s^2}\right] \times \left[A + \left[\frac{B}{N}\right] + \left[\frac{C}{N^2}\right] + \ldots\right], \quad (1)$$

resulted in values of A, B, and C of order -5, -50, and $+5000$, respectively. Thus five-digit accuracy in the shear modulus requires about 5000 particles. Data for a typical case, $\rho = 1.18$ and $kT/\epsilon = 1.00$, where ρ is the triangular-lattice number density, are shown in Fig. 1. See also Table I for the limiting values $G(0,\infty)$ and A.

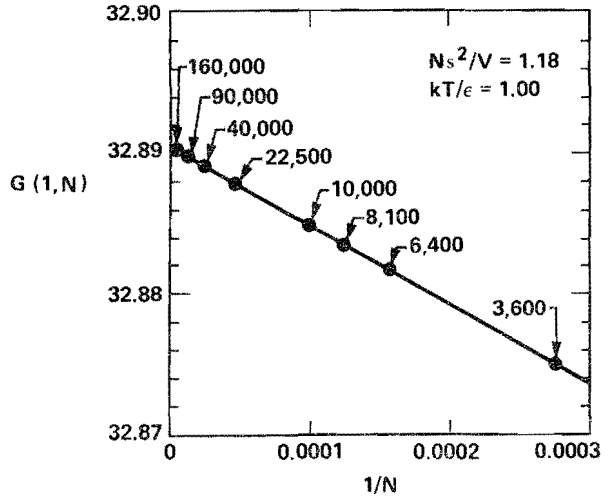

FIG. 1. Shear moduli for periodic quasiharmonic nearest-neighbor triangular-lattice Lennard-Jones crystals. The data shown correspond to crystals with from 3600 to 160 000 particles. The unit cells are all regular parallelograms.

The data leave no doubt that the quasiharmonic shear modulus for the triangular lattice varies as $1/N$ at low temperature. A correspondingly thorough investigation at temperatures near melting is impractical at present as a result of the excessive amount of time required for definitive Monte Carlo or molecular-dynamics simulations.

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[1]S. Toxvaerd, Phys. Rev. Lett. 51, 1971 (1983).
[2]W. G. Hoover, A. C. Holt, and D. R. Squire, Physica (Utrecht) 44, 437 (1969).

TABLE I. Quasiharmonic temperature dependence of the shear modulus in a nearest-neighbor triangular-lattice Lennard-Jones solid.

ρ	$G(0,\infty)$	A
$(4/3)^{0.5}$	31.177	−5.551
1.17	35.068	−5.142
1.18	37.807	−4.917

Toxvaerd Responds: The quasiharmonic calculations of the shear modulus, μ, by Hoover, Combs, and Massobrio in the preceding Comment[1] establish the size dependence of a two-dimensional (2D) solid at low temperatures, where μ is found to increase weakly ($\propto N^{-1}$) with increasing number of particles N. Near melting, however, another size dependence shows up.[2] Here the shear modulus is observed to decrease and additional data are in accordance with the logarithmic dependence of μ, found previously.

In order to determine the functional form of the size dependence of μ near melting we have performed additional calculations of μ for $N=100$ and $N=144$ with $\rho r_m^2=1.18$, and for the Weeks-Chandler-Andersen system considered in Ref. 1 The points are shown in Fig. 1, together with previously obtained values, and are plotted as a function of $\ln N$ (triangles) and N^{-1} (solid circles), respectively. The full line gives the result of the logarithmic plot, and the root-mean-square deviation (rms) from the straight line (full line) is 0.11. The corresponding rms deviation for the same points plotted as a function of N^{-1} is 0.39, and the points show a systematic deviation (from the dotted line). The statistical uncertainty per point is estimated to be 0.5 and so an N^{-1} dependence cannot be ruled out, but the $\ln(N)$ dependence gives a much better description of the size dependence. Also shown on the figure is the quasiharmonic result by Hoover, Combs, and Massobrio for the same density, but for another system. Their result is for a Lennard-Jones system with attractive forces. The attractive forces are observed to increase the shear modulus considerably and to stabilize the triangular 2D solid-state lattice so that the Lennard-Jones system melts at a somewhat lower density, $\rho r_m^2=1.137$.[3,4]

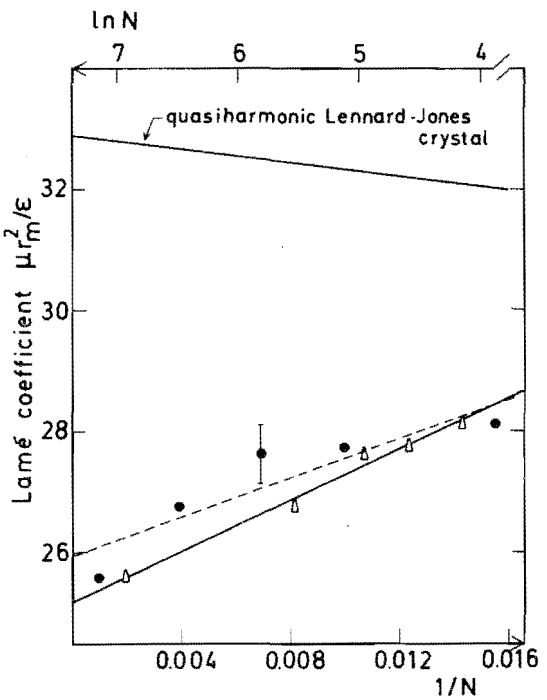

FIG. 1. Shear moduli, μ, for a 2D triangular lattice of repulsive Lennard-Jones particles near melting: $\rho r_m^2 = 1.18$, $kT/\epsilon = 1.00$. Triangles and full lines, data for the abscissa $\ln N$; full circles and dotted line, for the abscissa N^{-1}. The quasiharmonic result for a Lennard-Jones system (preceding Comment, Ref. 1) is also shown.

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