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Elastic Properties of Polycrystalline Solid Helium

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Abstract Recent experiments have shown that the shear modulus of solid helium undergoes a large temperature variation in the range 20 to 200 mK, possibly due to changes in the pinning of dislocations. In this note we report on computer simulations of the elastic properties of polycrystalline solid helium. We calculate how the elastic coefficients of a sample made up of a large number of randomly oriented grains are affected by the changes in the shear modulus c_{44} of the individual grains.

Keywords Solid helium · Supersolid

1 Introduction

In this paper we consider the elastic properties of polycrystalline solid helium. These properties are of interest in relation to the current investigations of a possible supersolid state of helium-4. Kim and Chan [1–3] performed torsional oscillator experiments with solid helium and found that below about 200 mK the period of the oscillator began to decrease suggesting that some fraction of the mass of the helium had decoupled and that a transition to a supersolid state had occurred. The existence of this effect has been confirmed by experiments in several other laboratories [4–10] but the magnitude of the effect has been found to vary significantly between the different experiments presumably because of variations in the way the solid helium samples were produced [11], a dependence on the amount of helium-3 impurity present [12], and differences in the sample geometry and the oscillator frequency.

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It has also been discovered that there are large changes in the shear modulus. Paalanen et al. [13] making measurements at 331 Hz found that the shear modulus at around 1 K was less than the low temperature limiting value ($T < 50$ mK) by a very large value, between 20 and 40%. It was proposed that at high temperatures dislocations are able to move rather freely, whereas at lower temperatures their motion is decreased because of pinning by helium-3 impurities. The binding energy of helium-3 to a dislocation is believed to be around 0.6 K [13]. More recently, Day and Beamish [14, 15] have made measurements by a different method and found an increase in the shear modulus starting below about 200 mK; they found a large increase in the range from 7 to 15% which varied from sample to sample [16]. Large changes have also been found by Mukharsky et al. [17] In a recent experiment, West et al. [18] have measured the period change in a very strong torsional oscillator where, given its estimated magnitude, a possible contribution of the helium stiffness to the resonance period should be negligible. They have concluded that the observed period change had to be due to a change in rotational inertia, not to the change in the helium stiffness. The obvious similarity between the elastic and the rotation anomalies indicates a relation between these two anomalies but, to our knowledge, its origin has not been established yet.

In many of the measurements just mentioned it is not certain whether the solid helium is a single crystal, is composed of a few crystalline grains, or has a grain size that is very small compared to the dimensions of the sample. The degree of disorder in the helium samples should depend on many parameters like the growth speed, the existence of temperature gradients in the cell, the nature of the liquid (normal or superfluid). Solid helium has a close-packed hexagonal structure (hcp) and its linear elastic properties are described by five elastic constants c_{11}, c_{12}, c_{13}, c_{33}, and c_{44}. The coefficient c_{44} is the ratio of shear stress to strain inside the basal plane so that it determines the velocity of purely transverse sound waves propagating along the c-axis ($v_T^2 = c_{44}/\rho$). For an hcp crystal it is natural to assume that the motion of dislocations is easiest in basal planes normal to the c-axis [19]. Thus, the effect of dislocation motion is to reduce the effective value of the elastic modulus c_{44}. For simplicity, we will assume that this is the only elastic coefficient that is modified. It is then interesting to ask to what extent a change in c_{44} will change the overall elastic properties of a polycrystalline sample. A polycrystal with a large number of grains that are randomly oriented will be elastically isotropic. The elastic properties can be described by two independent elastic constants, the effective "longitudinal modulus" $\tilde{c}_{11}$ and the shear modulus $\tilde{c}_{44}$. In this polycrystal, the transverse sound velocity is $v_T = \sqrt{\tilde{c}_{44}/\rho}$ and the longitudinal velocity is $v_L = \sqrt{\tilde{c}_{11}/\rho}$; the bulk modulus is $B = \tilde{c}_{11} - 4\tilde{c}_{44}/3$.

Of particular interest is the question what will be the macroscopic elastic properties of a solid when in each grain c_{44} becomes zero. The calculation below gives an upper bound for the possible softening of polycrystals when the shear modulus c_{44} of hcp grains decreases due to dislocation motion in their basal plane. One can also ask how $\tilde{c}_{44}$ depends on the relative magnitude of the grain size compared to the sample dimensions.

There are standard methods for the estimation of the elastic moduli of a polycrystal from a knowledge of the coefficients for a single crystal. The two classic methods are

Voigt [20] and Reuss [21] averaging. The Voigt average is based on the approximation that the strain field is uniform and for a crystal with hexagonal symmetry gives

$$\tilde{c}_{44} = \frac{1}{30}(7c_{11} - 5c_{12} - 4c_{13} + 2c_{33} + 12c_{44}). \tag{1}$$

The Reuss average takes the stress to be uniform and gives

$$\tilde{c}_{44} = \frac{15}{B[4(c_{11}+c_{12}) + 8c_{13} + 2c_{33}] + 6/c_{44} + 12/(c_{11}-c_{12})} \tag{2}$$

with

$$B = \frac{1}{c_{33}(c_{11}+c_{12}) - 2c_{13}^2}. \tag{3}$$

One can see that these formulas lead to quite different results in the limit as c_{44} goes to zero and thus cannot be considered to be useful in the present context. For Voigt averaging

$$\tilde{c}_{44} = \frac{1}{30}(7c_{11} - 5c_{12} - 4c_{13} + 2c_{33}), \tag{4}$$

and for Reuss averaging

$$\tilde{c}_{44} \approx \frac{5}{2}c_{44}. \tag{5}$$

There are more advanced averaging methods. For a recent discussion see the paper by Berryman [22].

2 Numerical Method

To calculate the effective shear modulus we consider a rectangular sample with sides L_x, L_y, L_z. In the x- and y-directions we take periodic boundary conditions. The sample is taken to have some number of grains N_g. To model the geometry of these grains we use Voronoi tessellations. We generate a set of N_g "grain points" with coordinates $\vec{r}_n = (c_x L_x, c_y L_y, c_z L_z)$ where c_x, c_y, c_z are random numbers in the range 0 to 1. For each grain point n we then add associated points displaced by vectors $(d_x L_x, d_y L_y, 0)$ where d_x and d_y are integers. A point $\vec{r}$ in the sample is then in grain n if it is closer to $\vec{r}_n$ (or to one of the points associated with $\vec{r}_n$) than for any other grain point. As an example, we show in Fig. 1 the grain structure that is obtained for a cube of side 1 cm that contains 50 grain points. The plot shows the intersection of grains with the plane $y = 0.5$ cm. The material in each grain is assigned a random orientation.

To calculate the shear modulus of the polycrystal we start with all parts of the sample undisplaced. We then give a unit displacement in the x-direction to the top surface ($z = L_z$) while holding points on the bottom surface ($z = 0$) fixed. The material in the sample is then allowed to relax to mechanical equilibrium and the average of the shear stress over the area of the top surface is calculated. To find the state of

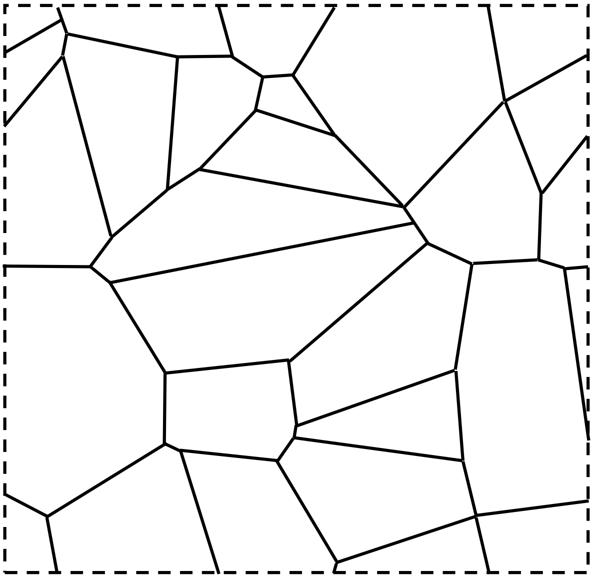

Fig. 1 Cross section showing the grain structure for a polycrystal cube of side 1 cm. The sample contains 50 grains. The *dashed lines* show the boundary of the sample

mechanical equilibrium we take the equations of linear elasticity and time develop the displacement using a finite difference method. For these calculations we take the elastic constants as measured by Greywall [23]. The values at the melting pressure of 25 bars are $c_{11} = 4.05$, $c_{12} = 2.13$, $c_{13} = 1.05$, $c_{33} = 5.54$, and $c_{44} = 1.24$ in units of 10^8 g cm^{-1} s^{-2}. It is assumed that these values are measured under conditions such that they are not appreciably affected by dislocation motion, i.e., it is assumed that the measurements are made at a temperature and sound frequency (10 MHz) such that dislocation motion is small and does not change the effective elastic constants appreciably. We now investigate the effect of reduction of c_{44} below the value just listed.

We first consider the effective shear modulus $\tilde{c}_{44}$ as a function of c_{44} for solid with grain size small compared to the sample dimensions. In these calculations the sample was a cube with side 1 cm containing 600 grains, and 125,000 mesh points were used for the finite difference simulation. Two sets of simulations were performed with different seeds for the random number generator that was used to set up the grain geometry and orientation. Results are shown in Fig. 2 along with the predictions of the Voigt and Reuss formulae. One can see that as might have been expected neither of these formulae is a good approximation when c_{44} becomes very small. The difference between the results from the two simulations gives an indication of the statistical errors resulting from considering a finite number of grains. One can see that when c_{44} is reduced from the value just given to zero the effective modulus $\tilde{c}_{44}$ is reduced to about 32% of the initial value.

We have performed a number of tests and found that, as expected, when the number of grains is large the result for the effective modulus is independent of the grain size.

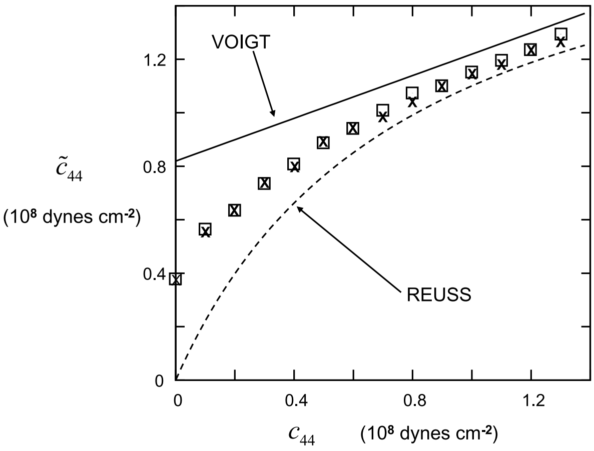

Fig. 2 The effective shear modulus $\tilde{c}_{44}$ as a function of c_{44} for a solid helium polycrystal containing 600 grains. The results of the two sets of simulations with different seeds for the random number generator are indicated by the *crosses* and *open squares*. The predictions of the Voigt and Reuss models are shown by the *solid* and *dashed lines*, respectively

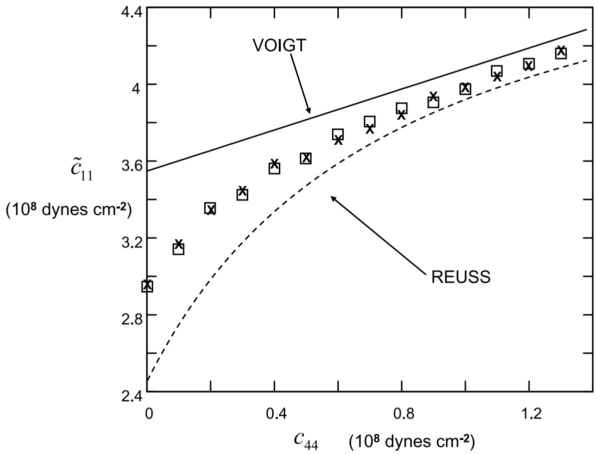

Fig. 3 The effective elastic modulus $\tilde{c}_{11}$ as a function of c_{44} for a solid helium polycrystal containing 600 grains. The results of the two sets of simulations are indicated by the *crosses* and *open squares*. The predictions of the Voigt and Reuss models are shown by the *solid* and *dashed lines*, respectively

In Fig. 3 we show similar results for the effective modulus $\tilde{c}_{11}$. One can see that the effect of decreasing c_{44} to zero is to reduce this "longitudinal velocity" modulus to 72% of the initial value.

In the experiments of Day and Beamish [14] the shear modulus is measured by forming a thin layer of solid helium between two piezoelectric transducers. By applying a voltage to one transducer a shear strain is produced in the solid helium. The second transducer is used to measure the shear stress. In this type of experiment it is possible that while the sample may contain many grains, each grain may extend from one transducer to the other. In this situation it is clear that for a given value of c_{44} the value of the effective modulus $\tilde{c}_{44}$ will depend on the ratio of the grain size to the spacing d between the transducers. Note that in this context by grain size Λ we mean the dimensions of the grains in the direction parallel to the surfaces of the transducers. We have performed a calculation to investigate what happens in this limit where $d \ll \Lambda$. The simulation was performed for a polycrystal with dimensions 1 cm by 1 cm by 0.03 cm with 60 grains. Thus, the average grain volume was 5×10^{-4} cm^3.

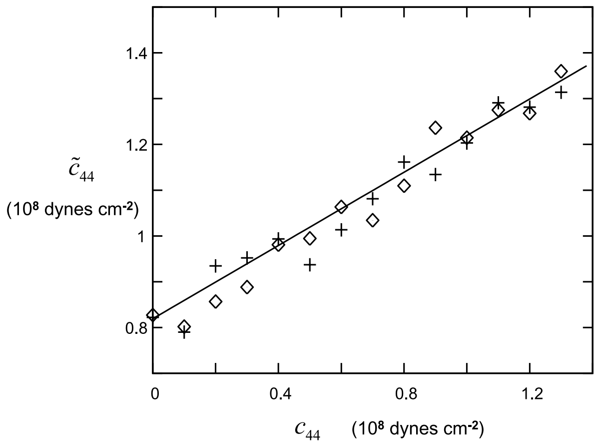

Fig. 4 The effective shear modulus $\tilde{c}_{44}$ as a function of c_{44} for a slab of solid helium polycrystal of thickness 0.03 cm. The grain size is such that most of the grains extend throughout the thickness of the slab. The results of the two sets of simulations are indicated by the *diamonds* and *crosses*. The prediction of the Voigt model is shown by the *solid line*

Since the grains can have a dimension in the z-direction of no more than 0.03 cm, this means that the average grain dimension in the x- and y-directions are approximately 0.13 cm. The results of two simulations with different random number seeding are shown in Fig. 4. The fluctuations in the results are larger here because the geometry of the sample forces us to run a simulation in which the number of grains is smaller. The effect of reducing c_{44} to zero is to decrease $\tilde{c}_{44}$ to 66% of the initial value. It can be seen that in this limit the results lie close to the predictions of the Voigt formula (1). This is to be expected in the limit $d \ll \Lambda$ because when this condition holds the displacement applied to the sample by the transducer results in the same elastic strain existing in each grain. It should also be noticed that if applied to the results by Day, Syshchenko and Beamish [15, 16] where a reduction by 7 to 15% of the average shear modulus was found, it would mean that c_{44} is reduced by between 18 to 39% of its normal value. Along with the same analysis, we predict that the shear modulus of a bulk polycrystal (not a thin slab) could be reduced to a lower value than measured by Day and Beamish in their slab geometry.

3 Summary

We have found that when c_{44} is decreased the fractional change in the effective shear modulus $\tilde{c}_{44}$ is larger than the corresponding change in the modulus $\tilde{c}_{11}$. The decrease when c_{44} goes from its value as measured ultrasonically down to zero is found to be 68% for $\tilde{c}_{44}$ and 28% for $\tilde{c}_{11}$. These numbers compared with the largest decrease in $\tilde{c}_{44}$ of 40% found by Paalanen et al. [13] and 7 to 15% found by Day et al. [14–16] The calculations reported here predict that for the same sample the percentage change in $\tilde{c}_{11}$ should be between 2 and 3 times less than the change in $\tilde{c}_{44}$; it would be interesting to make an experimental test of this prediction.

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