Topological defects and hcp nucleation in bcc Helium

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Abstract

We propose a new model for the nature of the nucleation of hcp from bcc Helium. The dynamic release of shear at the surface of the bcc-hcp phase boundary, sustains the simultaneous nucleation and growth of topological defects in the bcc phase. The topological defects are lines of dynamic shear in the bcc phase. The shear energy gain of this process balances the surface tension, as the growing hcp surface is quickly covered by many defect-loops. We show that this scenario gives better agreement with experiments, which differ with the classical theory of homogeneous nucleation by 6-10 orders of magnitude.

Key words: Solid Helium ; bcc-hcp nucleation; Topological defects ;

Recent experiments [1] have provided details of the hcp-bcc phase transition in ^{4}He. Around the higher temperature tri-critical point ($T_{c2} \simeq 1.778$K) the transition seems to be an internal solid-solid structural phase transition. The overcooling and overheating (or rather the overpressure) was found to be small compared to the expectations of the standard homogeneous nucleation model (HNM), which is off by 6-10 orders of magnitude.

Another example of non-classical nucleation, which occurs much below the HNM threshold, is the martensite transition in certain metals [2]. In these metals the easy nucleation is attributed to release of existing stress around static defects (dislocations) in the parent phase. This process can account for the process of bcc nucleating from the hcp phase. The hcp crystal from which the bcc forms is broken into many small grains, presenting a huge amount of structural dislocations, grain boundaries and internal stresses that can drive the nucleation of the bcc phase.

In the case of hcp nucleating from the bcc phase, static structural dislocations are unlikely to play a role, since bcc ^{4}He forms a single pure crystal. Rather we have previously shown the likely occurrence of topological defects in the bcc phase [3]. In the present work we propose that simultaneous nucleation of topological defects (in the bcc phase) reduces the energy of the hcp nucleus. Note that a similar discrepancy occurs in the case of the nucleation of solid Helium [4] from the superfluid phase, for which we also proposed a model incorporating topological defects (quantized vortices) [5].

In any solid there are structural dislocation lines and loops, which have a static stress field associated with them [6]. By contrast, the topological defects in bcc Helium introduce a relative phase change into the correlated atomic zero-point motion of the bcc ground-state [3,7]. In addition to linear defects, which have to terminate at the solid boundary, there are loop-defects of radius R, with energy

$$E_{loop} = \pi^2 E_0 \,(2R/a)\, ln(R/a) \tag{1}$$

where a, the core radius, is a free parameter in our model, and E_0 is the energy of the zone-boundary $T_1(110)$ phonon [7]. The smallest such loop defects costs an energy [7,3] $2E_0 \sim 14$K in ^{4}He. Recent experiments [8] indicate the existence of these topological defects in pure bcc ^{4}He. We also note that these excitations can play the role of vacancies in thermally activated mass diffusion [7], and have been observed

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by neutron scattering [9]. It is therefore natural to associate them with the atomic rearrangement which is involved in the bcc to hcp transition.

Due to the hybridization of the shear $T_1(110)$ phonon with the correlated zero-point motion, the topological defect lines have a dynamic shear field associated with them, oscillating with a frequency $E_0/\hbar$ [3,7]. The energy of a topological defect can be written in terms of the strain energy: $E_{defect} = E_0/V \int a^2(\nabla\xi)^2 dr$, where the strain gradient is $\nabla\xi \simeq (u/a)/r$ with the strain $\xi = u/a$, and u the transverse displacement. The shear modulus for the $T_1(110)$ displacements is given by E_0/V.

Following the treatment of a static dislocation loop [6], the energy of our loop-defect is reduced in an external shear-strain field $(\nabla\xi)_{ext}$

$$E'_{loop} = E_{loop} - P_{loop}(\nabla\xi)_{ext} \quad (2)$$

where we have defined an effective "momentum" of the loop-defect: $P_{loop} = \frac{\partial E}{\partial(\nabla\xi)} = \pi^2 E_0 \left(4R^2/a\right)$, in analogy with vortices in the superfluid [5]. For the external strain field $(\nabla\xi)_{ext}$ to reduce the energy of the topological defect (2), it has to be in-phase with the atomic oscillations at frequency $\omega_0 = E_0/\hbar$. This can occur if the bulk overpressure δP is released at the nucleating hcp boundary in the form of the softest Brilloin zone edge phonons, i.e. $T_1(110)$, corresponding to the rearrangement of a single atomic layer (Fig.1).

We now consider how does the creation of loop-defects compete with the energy cost of the surface tension. We estimate that the number of half-loops that can cover the hemispherical hcp nucleus is of the order [5]: $N_{vl} \sim (R/a_0)^2$ (Fig.1), where $a_0 \sim 1.5$Å gives the surface density of atoms of a single bcc unit-cell layer. The overall energy balance of the nucleating hcp phase is therefore

$$E_{tot} = N_{vl}E'_{loop} + E_{surf} \quad (3)$$

where $E_{surf} = 2\pi R^2\sigma$ is the surface tension energy.

We make a rough estimate of the size of the strain gradient field at the bcc-hcp boundary due to the released overpressure δP by equating the released overpressure energy in a unit cell $\sim \delta P a^3$ with the $T_1(110)$ shear energy $\sim m\omega_0^2 u^2/3$. The resulting strain gradient is then confined over a single unit cell: $\nabla\xi \simeq \sqrt{\frac{3\delta P}{a(m\omega_0^2)}}$. We find, using a value of $a = 5$Å, a critical overpressure of: $\delta P_c \simeq 1.0$bar. We find that the radius of the nucleating hcp at the critical overpressure is $R_c \sim 15$Å. The large number (~ 50) of defects on the surface of the hcp nucleus makes their energy nonadditive, unlike (3). Nevertheless, we assume that the nucleation is controlled by the energy barrier for a single loop-defect nucleation $\Delta E'_{loop}$. The reason is that once a single loop is created, in conjunction with the hcp nucleus, it will quickly multiply to cover the entire phase boundary if $E'_{loop} < 0$ (2).

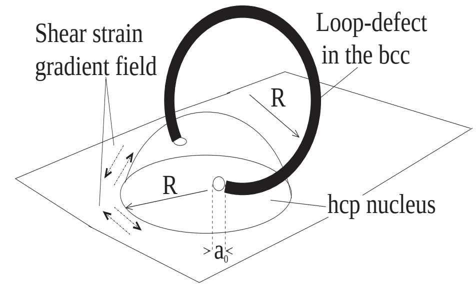

Fig. 1. A schematic picture of the simultaneous nucleation of topological loop-defects and a hcp nucleus.

Close to the critical overpressure the energy barrier is approximated by the power-law: $\Delta E \propto A\left(\delta P - \delta P_c\right)^{3/2}$. The experimental results for the bcc to hcp transition are [1]: $\delta P_c \simeq 1.05$bar, $A \simeq 15$K, while we find: $A \sim 450$K. The discrepancy of an order of magnitude is reasonable considering the rough approximations we made.

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