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Dislocation mediated shear instability of a 2D solid in a constant stress field

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Abstract. It is shown that the low-temperature behaviour of a pure 2D solid approaching plastic instability under a constant shear field can be modelled as a sort of *continuous phase transition* from a *metastable* equilibrium state to a *time-dependent* state of a flowing solid with vanishing shear modulus. With the difference that here the control parameter is the external shear strength and not the temperature, the mechanisms of the instability, in the high dislocation core energy regime, are the same invoked in the KTHNY theory of 2D melting: the dissociation and proliferation of dislocation dipoles with vanishing net Burgers vector. In this way, in two dimensions, some hidden similar statistical and structural properties of a melting solid and a plastically flowing one are put forward apart from the obvious analogies based on the common *fluid* behaviour. With the caution that the theory does not treat critical fluctuations properly, all the relevant thermodynamic functions exhibit *essential* singularities approaching the critical point. However, the excess specific heat is foreseen to be experimentally measurable within a stress range where fluctuations are negligible.

1. Introduction

The concepts of both order and thermodynamic stability of two-dimensional (2D) solids still remain partially open questions. In particular, 2D melting, in the absence of external fields, represents an intriguing problem in the modern theory of phase transitions. For a thorough critical analysis of the subject the reader is referred to the review paper [1] and to the references therein.

To clarify the theory of the peculiar low-temperature thermodynamic properties of a 2D solid in an external shear field, it is worth summarising the main results of the KTHNY theory [2, 3, 4] of 2D melting, for some similar mechanisms (see below) are probably operative in both cases. Following KTHNY theory, melting of 2D solids on an amorphous substrate is a continuous phase transition mediated by both dissociation and multiplication of topological defects pairs (pairs of edge dislocations with equal and opposite Burgers vectors) leading, above the critical temperature, to an anisotropic liquid (the hexatic phase). The solid phase possesses quasi-long-range positional order and long-range orientational order (topological order [2]), while the liquid phase has short-range positional order and quasi-long-range orientational order. From the thermodynamic point of view the main difference between an elastically isotropic solid and a liquid is that the solid has a non-vanishing shear elastic constant. This last quantity is operationally conceivable as the inverse of the (linear) shear strain response

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to an infinitesimal shear stress 'around a reference stress', divided by the stress itself. This concept can be applied to the case of interest here provided the 'reference stress' is finite and not zero. In this limited sense we see that both melting and the type of 'cold microcreep' treated in this paper lead, above some threshold, to 'states' with a vanishing shear elastic constant: while the 'solid' is flowing under the action of an external shear (easy glide) it can be considered as a sort of highly anisotropic 'fluid'.

With reference to the order of the melting transition, some experiments [5] and Monte Carlo simulations [6] seem to confirm the above theoretical predictions when the core energy of dislocation pairs (the self-energy of a pair with minimal distance in the lattice) is high. Otherwise a more usual first-order transition via nucleation and growth of grain boundaries seems to be more likely [7]. There are also theories not resorting to the concept of topological defects at all [8].

In this paper we study the statistical mechanics of a quite different phenomenon: the low-temperature microplastic instability of a 2D solid subjected to a critical shear field. Although this is not a phase transition (there is not a new stable equilibrium state beyond the 'critical point') we found that the instability (of an initially metastable equilibrium state) is mediated by both the dissociation and production of ever more mobile dislocation pairs as functions of the external stress level. The number of pairs and several thermodynamic functions show a 'critical behaviour', characterised by *essential singularities* in the very vicinity of the unstable point. Our approximate treatment of the phase approaching the instability cannot make one confident of the precise kind of divergency, but the qualitative statement that the instability starts and proceeds in a way similar to a continuous phase transition up to the 'critical stress value' seems to be generally true for the considered model Hamiltonian in the high core energy regime. Another similarity with the theory of melting is the renormalisation of the elastic shear modulus of the host solid due to the polarisability of dislocation pairs (reversible microplastic relaxation of shear stresses). The profound difference is that the renormalisation presented below is rather similar to a mean-field renormalisation and is not a recursive one based on scale invariance [3, 4].

The main approximations adopted in the paper are an expansion in fugacity of the dislocation grand partition function and the neglecting of dislocation climb. While the second approximation is an extremely good one at low temperature, the first is by no means obvious, its limit of validity residing in an (assumed) high value for the dislocation pair core energy. Going beyond this expansion could only be done in a numeric way [2].

2. The grand partition function of a 2D system of interacting dislocations in an external shear field

Our model system could describe both a 3D crystal containing infinite straight edge dislocations parallel to the z axis and a 2D solid lying, say, on the (x, y) plane, containing 'vector' point defects (2D edge dislocations [1]). We allow dislocation motion as well as production [9], so that the corresponding statistical problem will be tackled in the grand canonical ensemble. Yet, the assumption of low temperature is made in order to rule out complicated interactions between ordinary 'scalar' point defects (e.g. vacancies) and non-conservative motion of dislocations such as climb. The Hamiltonian for a dislocation pair with Burgers vector $\boldsymbol{b} = \pm b\hat{\boldsymbol{e}}_x$, in an *unstressed* elastically isotropic

solid†, reads [2, 10]:

$$H_0 = b^2 D \ln\left(\frac{r}{r_0}\right) - \tfrac{1}{2} b^2 D \cos(2\theta) + 2E_c \tag{1}$$

where r represents the modulus of the vector distance $\boldsymbol{r}$ between the two singularities and θ the angle $\boldsymbol{r}$ forms with the x axis (see figure 1), r_0 a short-range cut-off to avoid divergences; b is the modulus of a minimal Burgers vector of a dislocation (this last can lie along both x and y directions) in a square lattice of lattice parameter $a = b$, $2E_c$ is the core energy and D is related to the *bare* shear modulus μ and Poisson's ratio ν by

$$D = \frac{\mu}{2\pi(1-\nu)}. \tag{2}$$

When μ stands for the ordinary 3D shear modulus [energy/volume], H_0 and E_c are specific to a unit length (along z) of dislocation line. When instead μ is the 2D shear modulus [energy/surface], H_0 and E_c are directly energies. We shall consider only those complexions for which a *neutrality* condition $\sum_i \boldsymbol{b}_i = 0$ holds [4]. Within the fugacity expansion approximation used below this implies that no interactions between dislocations of non-parallel Burgers vectors are considered. We stress that inclusion of these higher-order effects would be very awkward due to the appearance of infinite self-energy terms in H_0 in the thermodynamic limit [3, 12]. From the macroscopic point of wiew the neutrality condition corresponds to assuming that there is no plastic bending of the solid as a whole [11].

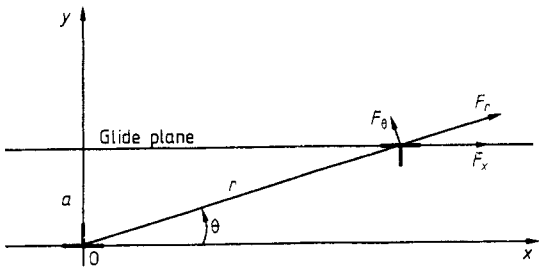

Figure 1. A dipole of edge dislocations of the *x family* (see §2). If climb is prohibited, only the x components (glide) of internal forces are effective.

Let us now consider the effect of a uniform external shear field (only the components $\sigma_{yx} = \sigma_{xy}$ of the stress tensor are not vanishing). The corresponding *configurational* forces [12] acting on dislocations are given by the Peach–Koehler–Weertman formula [10]. By integration we get, still for a dislocation pair with $\boldsymbol{b} = \pm b\hat{\boldsymbol{e}}_x$, an additional contribution to H_0:

$$H_s = -b\sigma_{xy} r \cos\theta \tag{3}$$

† This is the correct elastic Hamiltonian only if the underlying 2D Bravais lattice is hexagonal [11]: in the case of the simple square lattice used here it is only a very frequent and good approximation. The same pair Hamiltonian has been used in the KTHNY theory of melting.

where we consider just glide in the x direction. Pairs with $\boldsymbol{b} = \pm b\hat{\boldsymbol{e}}_y$ are treated similarly in an additive way, cross terms being absent in the considered approximation (see above and [4]).

In the frame of linear elasticity $H_0 + H_s$ singular contributions for each dislocation pair of each family must be added to a non-singular [3] elastic Hamiltonian describing, in the long-wavelength limit, the uncoupled phonon excitations of the solid. This last Hamiltonian is written in terms of symmetrised elastic displacement gradients (the curl-free part [3, 9, 11] of the elastic strains) and possesses full elastic isotropy and continuous orientational symmetry. The unstressed 2D solid phase at low temperature is a much less symmetric phase (see above) in which topological order is compatible with an infinitesimal number of *spontaneous* dislocation pairs (disclination quadrupoles [3]) excitations described by H_0. H_s describes *field-driven* polarisation of dislocation 'molecules' and their subsequent dissociation, multiplication and mobilisation leading to destruction of topological order and time invariance (flowing plastic solid)†.

Taking now as new variables the separation in the glide direction $x = r\cos\theta$ and the distance a between two parallel planes, we get the *unidimensional* Hamiltonian

$$H(x,a) = Db^2 \ln\left(\frac{(x^2+a^2)^{1/2}}{r_0}\right) - \frac{1}{2}Db^2\,\frac{x^2-a^2}{x^2+a^2} - b\sigma_{xy}x. \tag{4}$$

The normalised Hamiltonian H/Db^2 is plotted in figure 2 for increasing values of the normalised shear $\tau = \sigma_{xy}/D$. Study of the surface $H = H(x,a)$ gave no evidence of minima with respect to a, which must be taken as just a parameter and not a dynamic coordinate from now on because we exclude climb motions‡.

The Hamiltonian (4) enters the expression of the grand partition function Q_x we have expanded up to second order in fugacity $f = \exp(-\beta E_c)$ [2, 13]

$$Q_x = 1 + \frac{A}{2b^2}f^2 \int \exp(-\beta H(x,a))\mathrm{d}x + \mathrm{O}(f^4) \tag{5}$$

where A is the area of the system and from now on x is measured in units of $b : x \to x/b$. The total grand partition function Q for both dislocation dipole families (see above) is $Q = Q_xQ_y + \mathrm{O}(f^4) = Q_x^2 + \mathrm{O}(f^4)$. In this way Q is proportional to the sum of the probabilities of seeing either no dipoles or only one x-dipole or only one y-dipole at the same time.

In (5) the original lattice sum has been replaced by an integral because we are interested in the long-wavelength properties of the system.

In the thermodynamic limit [2] the above grand partition function Q is formally divergent, revealing an *infinite plastic susceptibility* with respect to an external shear. However, the relative minimum at finite x in $H(x,a)$ shown in figure 2 makes practically time-independent (metastable) states possible at low shears (see the next section).

3. Metastable states and parabolic approximation

As we see in figure 2, for $\tau = 0$ the dipole Hamiltonian has the typical form of a bistable potential, corresponding to a couple of equally probable complexions. These

† The complete Hamiltonian (1) + (3) has already been considered in the KTHNY theory of 2D melting but only to compute the 'polarisability' of the gas of dipoles around *zero stress*.

‡ The surface H also showed a monotonic increase with respect to a, suggesting $a = b$ as the most probable value at equilibrium. A later variational check showed the same increase in the grand canonical potential Ω itself.

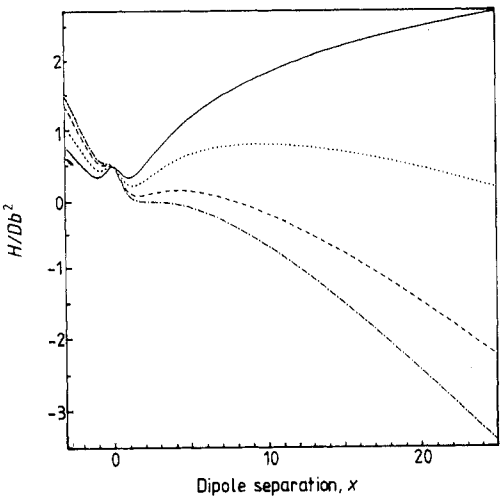

Figure 2. The complete Hamiltonian of a dislocation dipole. The activation energy $\Delta E(\tau)$ is the energy difference between the right minimum and the maximum (see figure 3). The Hamiltonian coincides with potential energy because the effective mass of dislocations is negligible in equilibrium problems. Full curve, $\tau = 0$; dotted curve, $\tau = 0.1$; broken curve, $\tau = 0.2$; chain curve, $\tau = 0.25$.

are two equivalent dipoles with $\theta = \pi/4$ and $\theta = 3\pi/4$ (figure 1). The introduction of an external shear breaks this symmetry and brings about major changes in the physics of the problem. First, the abrupt appearance of a 'third minimum of infinite depth at $x = \infty$' in $H(x)$ turns the system from a stable into a metastable one. No matter how long it will take to get through the potential barrier, $x = \infty$ will eventually be reached and the system will dissociate. The outcome is a time-dependent state featuring irreversible plastic flow. Strictly speaking, equilibrium statistical mechanics cannot correctly be used to study such a transition. Kinetics methods should be required (e.g. the solution of the Fokker–Planck equation for dislocation transport). In this paper we shall use the approximate alternative equilibrium approach known as 'parabolic approximation' [14]. A look at figure 2 serves to illustrate the spirit of the approximation. Increasing τ the position $\bar{x}$ of the relative right minimum shifts towards larger x while the curvature of $H(\bar{x})$ goes to zero. Such a change is seen to happen *continuously* and to wind up in a 'critical state'† for a computed value $\tau = 0.25$ (inflection point in figure 2). Beyond this value no minima are shown any more: dislocations are free to move at any temperature. Here we consider the shear as the *control parameter* and the temperature just as a 'source' of fluctuations.

Comparison between the activation energy (the height of the barrier $\Delta E(\tau)$ in figure 3) and the 'thermal energy' $k_B T = \beta^{-1}$ becomes crucial for the parabolic approximation to be tenable: a tall barrier 'deceives' the system and makes it 'miss' the much more favourable accommodation for $x = \infty$. If this is the case, $H(x)$ can be confused with its Taylor expansion up to second order around $\bar{x}(\tau)$. We have checked the condition $\Delta E \geq 2k_B T$ for room temperature Al [15] and found it quite satisfied up to 80 % of the critical shear. As in the case of a mean-field theory, critical fluctuations

† The term 'critical' will always appear in quotes throughout this paper since we are not dealing with a continuous *phase transition* but with the *soft instability* of a *metastable* state.

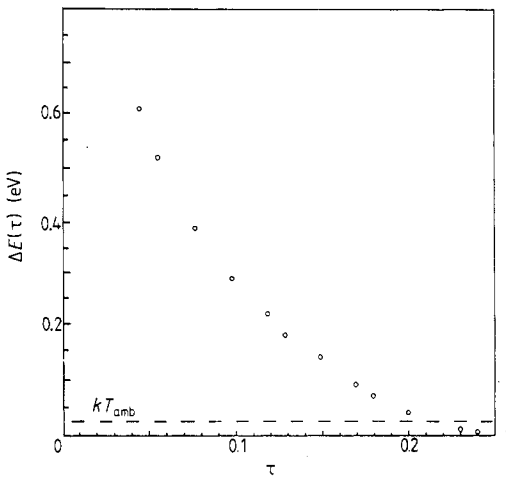

Figure 3. Activation energy $\Delta E(\tau)$ plotted against τ compared with room temperature thermal energy.

cannot be treated properly by the parabolic approximation (see below). Because it is not possible to write down exact practical analytical expressions for $\bar{x}(\tau)$, which is the root of the fourth-order algebraic equation

$$x\,\frac{x^2-a^2}{(x^2+a^2)^2}=\tau \tag{6}$$

we have solved (6) numerically with high precision and then fitted the numerical solution to the simple 'critical' relationship

$$\bar{x}(\tau)=x_c-(x_c-a)\left(\frac{\tau_c-\tau}{\tau_c}\right)^{\alpha} \tag{7}$$

where $a=1$, $x_c=2.414\,213$ and $\alpha\simeq 1/3$. The analytic approximation (7) turns out to fit quite well the numerical solution for any τ and especially near its critical value. We can now write the parabolic approximation for H as

$$H(x)\simeq H(\bar{x})+\frac{1}{2}\left(\frac{\mathrm{d}^2H}{\mathrm{d}x^2}\right)_{x=\bar{x}}(x-\bar{x})^2 \tag{8}$$

where $H(\bar{x})$ and the second derivative of H at $\bar{x}$ are easily computable from (4) and (7).

4. 'Critical' thermodynamic behaviour

The grand canonical potential suitable for our problem is, for a given area of the system, a natural function of temperature, shear and core energy, and can be written as

$$\Omega=F+2E_c\langle N\rangle-2A\sigma_{xy}\langle\epsilon_{xy}\rangle \tag{9}$$

where F is the Helmholtz potential, $\langle N \rangle$ is the mean number of dislocation dipoles and $\langle \epsilon_{xy} \rangle$ is the mean dislocation shear strain conjugated to σ_{xy} and microscopically conceivable as:

$$\langle \epsilon_{xy} \rangle = \frac{b}{2A} \left\langle \sum_{i=1,N} x_i \right\rangle \tag{10}$$

where $\langle \ldots \rangle$ means the grand canonical average, N is the fluctuating number of dipoles and bx_i is the fluctuating 'dipole moment' of each dislocation pair. $-2E_c$ plays the formal role of a chemical potential for dislocation pairs.

Using the grand canonical normalisation condition [13], we obtain the usual relation between Ω and Q: $\Omega = -k_B T \ln Q$ which, in our case, reads

$$\Omega = -k_B T \ln \left(1 + \frac{A}{b^2} f^2 \int \exp(-\beta H(x, a)) \, dx \right). \tag{11}$$

Evaluating the Gaussian integral in (11) we find

$$\Omega = -k_B T \ln \left[1 + \frac{A}{b^2} f^2 \exp(-\beta H(\bar{x})) \left(\frac{2\pi}{\beta H''(\bar{x})} \right)^{1/2} \right]. \tag{12}$$

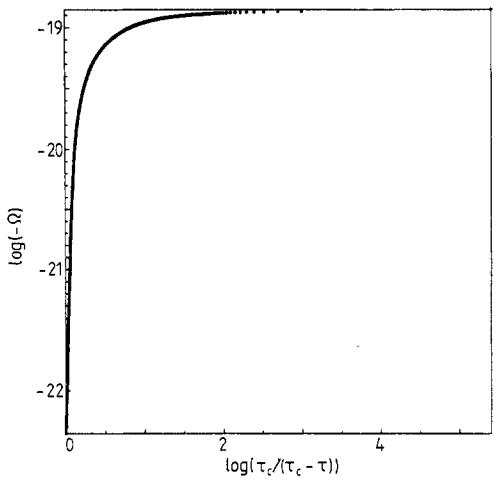

Figure 4. The grand canonical potential plotted against shear. The logarithmic divergency is clearly visible.

Figure 4 shows the *logarithmic* divergency of Ω as $\tau \to 0.25$ It is now straightforward to compute all the relevant thermodynamic functions from the definition (9) of Ω:

$$S = -\left(\frac{\partial \Omega}{\partial T} \right)_{E_c, \sigma} \qquad \langle N \rangle = \frac{1}{2} \left(\frac{\partial \Omega}{\partial E_c} \right)_{T, \sigma} \qquad \langle \epsilon_{xy} \rangle = -\frac{1}{2A} \left(\frac{\partial \Omega}{\partial \sigma_{xy}} \right)_{T, E_c} \tag{13}$$

where S is the entropy. From (13) the heat capacity at constant shear C_σ and the inverse of the shear modulus μ_D of the dislocation subsystem can be derived by further differentiation:

$$C_\sigma = T \left(\frac{\partial S}{\partial T} \right)_{E_c, \sigma} \qquad \frac{1}{\mu_D} = \left(\frac{\partial \langle \epsilon_{xy} \rangle}{\partial \sigma_{xy}} \right)_{T, E_c} \tag{14}$$

We are now in a position to set an intriguing 'duality' between 2D melting (high temperature, no stress) and 2D plastic instability (low temperature, constant shear stress). At high shears dipole production gets thermodynamically favoured as well as larger dipoles moments. Both the proliferation and dissociation of dislocation dipoles induce divergency of all the above thermodynamic functions. Very near the 'critical point' all the above quantities display *essential* singularities which must be partly considered as artefacts of the parabolic approximation.

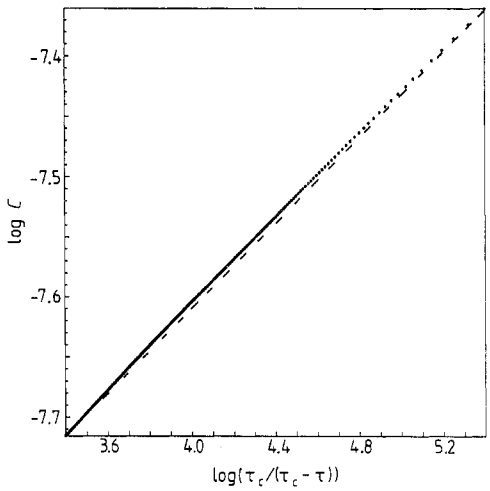

Figure 5. Essential singularity of specific heat. The bisectrix has been drawn to show that the slope of the log–log plot is not constant. This is true at any scale near the critical shear.

Figure 5 shows the excess heat capacity divergency for $\tau \to 0.25$. We notice that in the KTHNY theory of 2D melting also, the specific heat exhibits a (different) type of essential singularity as a function of temperature.

Considering an area of 1 cm^2, at $\tau = 0.2$, where the above approximation is still tenable, the excess heat capacity turned out to be approximately 19% of the corresponding quantity for the perfect solid computed from the 2D Dulong and Petit law ($2k_B$ per atom).

From the data shown in figure 6 the behaviour of the renormalised shear modulus $\mu_R = \mu\mu_D/(\mu + \mu_D)$ can be obtained, from which its vanishing for $\tau \to 0.25$ is deduced although this is hardly seen with any finite numerical precision because μ_D (see figure 7) is much bigger than μ except in the immediate neighbourhood of the critical shear. This means that the thermal warning signs of the instability should be more easily visible, and better represented by the present theory, than the mechanical ones.

5. Conclusions

The physics of melting and of plasticity of solids have always been recognised to have some similarities. From the macroscopic point of view the two phenomena share the common *fluid* response to shear stresses albeit in the case of melting the probe shear is just a virtual one [3] and in the case of plasticity the fluidity is often far from being perfect.

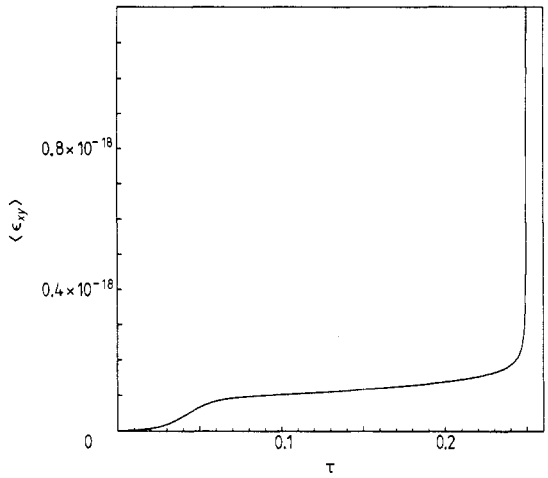

Figure 6. Dislocation strain response plotted against shear. Note the sharpness of the transition.

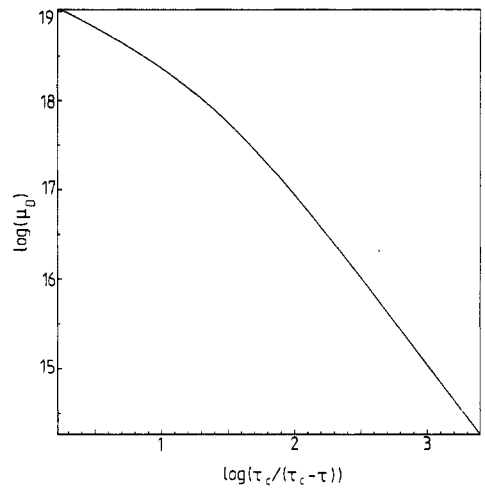

Figure 7. Dislocation shear modulus plotted against shear. The modulus vanishes at the critical stress $\tau = 0.25$.

Dislocation theory offers a common microscopic mechanism for both cases but in 3D systems the line nature of dislocations makes any rigorous attempt at a unified view hopeless [10]. In two dimensions the topology is much simpler and dislocations are *thermodynamic defects*. Yet, the very peculiar nature of long-range order in 2D, firstly clarified by Kosterlitz and Thouless [2] and later by Halperin and Nelson [3], makes the physics not trivial.

In this preliminary paper we have shown the singular nature of the thermodynamic properties of a pure 2D solid on a smooth substrate under a constant shear. In particular, the excess specific heat exhibits a rather gradual and significant variation in a stress range where fluctuations are negligible. The envisaged mechanisms for the plastic instability are seen to be operating in the same way in the KTHNY theory of 2D melting: proliferation and dissociation of dislocation dipoles.

Acknowledgments

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