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Viscoelasticity from a Microscopic Model of Dislocation Dynamics

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It is shown that the dynamics of a two-dimensional crystal with a finite concentration of dislocations, as well as vacancy and interstitial defects, is governed by the hydrodynamic equations of a viscoelastic medium. At the longest length scales the viscoelasticity is described by the simplest *Maxwell* model, whose shear and compressional relaxation times are obtained in terms of microscopic quantities, including the density of free dislocations. At short length scales, bond orientational order effects become important and lead to wavevector dependent corrections to the relaxation times.

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I. INTRODUCTION

Experimental [1–4] and numerical [5–9] studies of the dynamics of driven disordered media, such as vortex arrays in type-II superconductors and charge density waves in metals, have clearly indicated that when the disorder is strong these systems exhibit a spatially inhomogeneous plastic response upon depinning, without long wavelength elastic restoring forces [10]. In this plastic regime dislocations proliferate due to the interplay of drive, disorder and interactions, and the system is broken up in fluid-like regions flowing around solid regions [6]. It was proposed recently [11] that a description of shear deformations in this plastic regime may be obtained by focusing on the dynamics of coarse-grained degrees of freedom (the solid-like regions) and replacing the elastic couplings of local displacements with viscoelastic couplings of local velocities. It was found that the simplest, Maxwell, model of viscoelasticity yields interesting features, such hysteretic depinning and switching, which have also been observed in experiments. The local viscoelastic couplings were introduced as an ad hoc way of mimicking the presence in the system at any given time of unbound dislocations, whose motion is in turn responsible for plastic slip.

In this paper we provide some justification to the model studied in Ref. [11] by showing that the dynamics of a two-dimensional crystal with a finite concentration of *annealed* free dislocations, as well as vacancy and interstitial defects, is governed by the hydrodynamic equations of a viscoelastic medium (with hexatic order). Starting with the hydrodynamic equations for a two-dimensional solid with finite concentrations of dislocations, vacancies and interstitials obtained some time ago by Zippelius, Halperin and Nelson [12] (ZHN), we show that such equations can be recast in the form of hydrodynamic equations for a viscoelastic medium, with a Maxwell form for the nonlocal transport coefficients [13].

It has of course long been recognized that the creation and motion of dislocations are the main mechanism by which a crystal undergoes plastic deformations [14,15].

A number of efforts [16,17] have been made to describe the motion of dislocations through crystalline solids and relate the plastic strain rate to the dislocation dynamics. There has also been work specifically on the effect of dislocation motion on linear and nonlinear stress relaxation in a two-dimensional crystal [16], where it was shown *for a particular geometry* that the crystal responds viscoelastically when free dislocations are present. Our work generalizes this by obtaining equations that describe the viscoelastic response of a two-dimensional solid to stresses in an *arbitrary geometry*. The equations incorporate viscoelastic effects in the response to both shear and compressional deformations, and have precisely the structure of the viscoelastic equations for a simple viscous fluid [18]. Furthermore, our derivation yields expressions for the (Maxwell) relaxation times for shear and compression in terms of microscopic parameters.

Of course, in the presence of *quenched* disorder and drive, dislocations are continuously generated and healed in the system. Furthermore, they are not always free to move and relax a local stress as they may be pinned by disorder. For these reasons one may question the assumption behind the model introduced in Ref. [11], namely that the plastic response of extended media driven over strong quenched disorder at zero temperature may be described at large scale by the same equation that govern the stress relaxation due to the motion of annealed dislocations. At best, the effective density of "free" dislocations that can relax local stresses will be a strong function of the applied driving force, disorder, and possibly time. As shown in Ref. [11], the depinning of a driven viscoelastic medium does, however, exhibit a number of features seen in experiments, namely memory effects and coexistence of weakly and strongly pinned degrees of freedom. It does, therefore provide a useful starting model for the description of the complex dynamics of these systems.

Finally, it should be pointed out that crystals with annealed dislocations and simple viscous fluids are not the only examples of viscoelastic media. Linear viscoelasticity is of course one of the distinctive properties of complex and polymeric fluids, that can fill containers of any

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shape and yet may shrink like rubber when stretched and released quickly. Molecular theories of viscoelasticity for complex fluids have been developed by various methods and there is a vast literature on the subject [19].

II. SUMMARY OF MAIN RESULTS AND OUTLINE

It is well known that a dense fluid has insufficient time to flow in response to a high frequency strain rate, but instead reacts elastically, as a solid would [20]. This leads to the appearance in the fluid of propagating shear waves, with an associated peak at nonzero frequency in the spectrum of transverse current fluctuations. Such viscoelastic effects are easily incorporated phenomenologically into the hydrodynamic description of fluids [13]. If a shearing force is applied to a fluid yielding a stress σ_{xy}, the local strain at each point can be expressed in terms of derivatives of the displacement field $\mathbf{u}$ at that point. In a steady-state situation the flow is purely viscous and the stress is proportional to the local rate of strain,

$$\sigma_{xy} = \eta \frac{\partial}{\partial t}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right) , \tag{1}$$

where η is the shear viscosity. By contrast, if the force is applied suddenly, the instantaneous displacement is related to the stress via a typical elastic stress-strain relation,

$$\sigma_{xy} = \mu\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right) , \tag{2}$$

where μ is the instantaneous (high-frequency) shear modulus. An interpolation between these two forms yields the Maxwell model of viscoelasticity, where the stress-strain rate relation takes the form of a differential equation,

$$\frac{\partial \sigma_{xy}}{\partial t} + \frac{\sigma_{xy}}{\tau_M} = \mu\left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x}\right) . \tag{3}$$

The local flow velocity, $\mathbf{v}$, of the constituent particles is identified as the rate of change of the displacement, $\mathbf{v} = \partial_t \mathbf{u}$, and $\tau_M = \eta/\mu$ is called the Maxwell relaxation time. The Maxwell model of viscoelasticity given by Eq. (3) yields elastic response to high frequency shearing forces ($\omega\tau_M >> 1$) and viscous response at low frequency ($\omega\tau_M << 1$).

In general, viscoelastic effects are present in the response to both shear and compression and can be described by modifying the hydrodynamic equations of a fluid by introducing nonlocal (in space and time) thermodynamic quantities and transport coefficients. This can be done phenomenologically through the use of frequency sum rules as constraints, or can be formulated more systematically by deriving such equations via formal projection operator methods or kinetic theory techniques [18,20]. In its simplest realization this approach yields the Maxwell model of viscoelasticity.

In this paper we show that the hydrodynamic equations for a two-dimensional solid with a finite concentration of free dislocations proposed by ZHN are equivalent to a set of hydrodynamic equations for a simple fluid (with hexatic order), with a Maxwell-type stress-rate of strain relation. For convenience, we define a symmetrized strain rate, v_{ij}, as

$$v_{ij} \equiv (\partial_i v_j + \partial_j v_i)/2$$
$$= \tilde{v}_{ij} + \frac{1}{2}\delta_{ij}v_{kk} , \tag{4}$$

where we have separated the traceless part $\tilde{v}_{ij}$ and the trace $v_{kk} = \nabla \cdot \mathbf{v}$. It is also useful to separate the stress tensor σ_{ij} into its traceless part and its trace, i.e.,

$$\sigma_{ij} = \tilde{\sigma}_{ij} + \frac{1}{2}\delta_{ij}\sigma_{kk} . \tag{5}$$

We find that, at long wavelengths, the traceless part of the stress tensor is related to the strain rate according to

$$\frac{\partial \tilde{\sigma}_{ij}}{\partial t} + \frac{\tilde{\sigma}_{ij}}{\tau_s} = 2\mu\tilde{v}_{ij} , \tag{6}$$

where τ_s is the shear relaxation time, which is obtained in terms of microscopic parameters (see Eq. (35) below). Equation (6) is precisely of the Maxwell form. If the product $\mu\tau_s$ is identified with the shear viscosity η of the fluid, Eq. (6) yields viscous flow in response to low frequency shearing forces. It also describes the fact that a liquid always flows in response to a steady shear.

In contrast, even a liquid has a finite low frequency compressional modulus, that is, it resists elastically low frequency compressional deformations. The trace of the stress tensor, σ_{kk}, contains both reversible contributions proportional to pressure changes arising (assuming temperature fluctuations are negligible) from the fractional change in volume and irreversible and dissipative contributions proportional to velocity gradients. It can be written as

$$\sigma_{kk} = -2B_0\frac{\delta n}{n_0} + \sigma_{kk}^{\text{dis}} , \tag{7}$$

with δn the deviation of the density from its equilibrium value n_0, and B_0 the low frequency bulk modulus of the solid (which generally depends on the density of vacancies and interstitials defects). To a good approximation B_0 is also the compressibility of the liquid phase [21]. We find that the dissipative part σ_{kk}^{dis} of the stress tensor is related to the local rate of strain via the equation

$$\frac{\partial \sigma_{kk}^{\text{dis}}}{\partial t} + \frac{\sigma_{kk}^{\text{dis}}}{\tau_b} = -2(B_\infty - B_0)\frac{\delta n}{n_0} , \tag{8}$$

where B_∞ is the high frequency compressional modulus of the solid in the absence of defects. At high frequency

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defects do not have time to respond to an applied force and therefore do not contribute to the elastic constants. Finally, τ_b is the compressional relaxation time, which again is given below in terms of microscopic quantities. Both relaxation times, τ_s and τ_b are inversely proportional to the density of free dislocations, n_f. As a result, they both diverge as the melting temperature T_m of the two-dimensional solid is approached from above as [21,22]

$$\tau_{s,b} \propto \exp(b/(T - T_m)^\alpha) , \qquad (9)$$

with $\alpha = 0.36963$. At the longest length scales, the bulk viscoelasticity described by Eq. (8) is due solely to dislocation *climb*, while the shear viscoelasticity is due to both dislocation climb and *glide*. Dislocation climb which requires the creation of vacancies and interstitials, proceeds more slowly than dislocation glide which does not involve a change in particle number. For this reason, $\tau_b \gg \tau_s$, in general.

Of course, the 2d solid does not melt directly into a isotropic liquid at T_m, rather it enters the hexatic phase, where it has only short-ranged translational order, but retains quasi-long-ranged bond orientational order (BOO). At the longest length scales, the presence of BOO does not affect the stress-rate of strain relations. When terms of higher order in the gradients of the hydrodynamic fields are included, the existence of BOO becomes apparent and modifies the stress-strain rate relations at finite length scales, as discussed in Section V below. In particular, this gives wavevector-dependent corrections to τ_s and τ_b, corresponding to a distribution of relaxation times.

The rest of the paper is organized as follows. In Section III we review the hydrodynamic equations for a two-dimensional solid with vacancy and interstitial defects [12]. In Section IV the viscoelastic stress-rate of strain relations are derived in the longest length scale regime, and expressions for the long-wavelength viscoelastic memory times are presented. In Section V the effects of incorporating higher order gradients are investigated, including the wavevector dependent corrections to τ_s.

III. ZHN HYDRODYNAMICS OF A SOLID WITH DISLOCATIONS

We begin by reviewing the hydrodynamics of the solid phase, following Refs. [12], [23] and [24]. We consider a two-dimensional hexagonal crystal with a finite density of vacancies and interstitials. As pointed out by Martin [23], incorporating a finite density of point defects is crucial to properly distinguish between local lattice deformations and local changes in the number density. For simplicity, temperature fluctuations are neglected in all of the following.

In the absence of dislocations, the equations for conservation of density, $n(\mathbf{r}, t)$, momentum, $\mathbf{g}(\mathbf{r}, t)$, and net defect density, $n_\Delta(\mathbf{r}, t)$, i.e., density of interstitials minus density of vacancies, and the equation of motion for the displacement field, $\mathbf{u}(\mathbf{r}, t)$, can be written as

$$\frac{\partial n}{\partial t} = -\frac{1}{m} \nabla \cdot \mathbf{g} , \qquad (10a)$$

$$\frac{\partial g_i}{\partial t} = \partial_j \sigma_{ij} , \qquad (10b)$$

$$\frac{\partial n_\Delta}{\partial t} = -\nabla \cdot \mathbf{j}^\mathbf{\Delta} , \qquad (10c)$$

$$\frac{\partial \mathbf{u}}{\partial t} = \frac{\mathbf{g}}{mn_0} - \frac{\mathbf{j}^\mathbf{\Delta}}{n_0} , \qquad (10d)$$

where m is the mass of the constituent particles and n_0 is the average number density.

These conservation laws must be completed with constitutive equations for the two fluxes, the momentum flux or stress tensor, $\sigma_{ij}(\mathbf{r}, t)$, and the defect current, $\mathbf{j}^\mathbf{\Delta}(\mathbf{r}, t)$. Assuming purely relaxational dynamics for the defects, $\mathbf{j}^\mathbf{\Delta}$ is given by

$$\mathbf{j}^\mathbf{\Delta} = -\Gamma n_0 \nabla p_d , \qquad (11)$$

where Γ is a constant kinetic coefficient and p_d is the defect pressure,

$$p_d = \chi^{-1} \frac{\delta n_\Delta}{n_0} + \gamma \nabla \cdot \mathbf{u} , \qquad (12)$$

with χ a susceptibility proportional to the sum of the equilibrium densities of vacancies and interstitials, and γ a constant associated with the coupling between changes in defect density and bulk distortions in the lattice. The constitutive relation for the stress tensor, σ_{ij}, is

$$\sigma_{ij} = 2\mu w_{ij}^s + \lambda w_{kk}^s \delta_{ij} + \gamma (\delta n_\Delta / n_0) \delta_{ij} , \qquad (13)$$

where $w_{ij}^s = (w_{ij} + w_{ji})/2$ is the symmetric part of the strain tensor w_{ij}, given by

$$w_{ij} = \partial_i u_j . \qquad (14)$$

The coefficients μ and λ are the Lamé constants. We note that the equilibrium bulk modulus, B_0, of the solid is defined in terms of the response to a static isotropic compression as $B_0 = \left[-\frac{1}{A} \frac{\delta A}{\delta p} \right]^{-1}$, with A the area of the crystal. In the presence of defects it is then given by

$$B_0 = \frac{\mu + \lambda - \gamma^2 \chi}{1 + (\mu + \lambda + 2\gamma)\chi} , \qquad (15)$$

On the other hand, if one were to measure the bulk modulus on time scales long compared to the elastic relaxation time, but short compared to the defect diffusion time, the effective bulk modulus, denoted by B_∞, would be

$$B_\infty = \mu + \lambda , \qquad (16)$$

corresponding to the purely elastic contribution obtained in the absence of defects. In a finite-frequency measurements, the value $B_\infty > B_0$ is reached at sufficiently high frequency. Finally, changes in the defect density can be related to changes in the overall density and bulk strains in the lattice, as

$$\delta n = \delta n_\Delta - n_0 w_{kk} \; , \qquad (17)$$

where $\delta n = n - n_0$ and $\delta n_\Delta = n_\Delta - n_0^\Delta$ are the deviations of the density and defect density from their equilibrium values, respectively.

In the presence of dislocations, it is no longer possible to define a continuous single-valued displacement field, **u**. One can define a single-valued, but discontinuous displacement field by introducing cuts at the location of the dislocations. The strain field $w_{ij} = \partial_i u_j$ is still single valued and continuous, except at the location of the dislocations, and it satisfies

$$\epsilon_{ki}\partial_k w_{ij} = a_0 B_j \; , \qquad (18)$$

where a_0 is the lattice spacing, ϵ_{ij} the antisymmetric unit tensor, and $\mathbf{B}(\mathbf{r},t)$ is the Burgers-vector charge density. For a set of M free dislocations at discrete points $\{\mathbf{R}_\nu\}$, $\nu = 1,2,...,M$, with Burgers vector $\mathbf{b}_\nu$, it is given by

$$\mathbf{B}(\mathbf{r},t) = \sum_{\nu=1}^{M} \mathbf{b}_\nu \delta(\mathbf{r}-\mathbf{R}_\nu) \; . \qquad (19)$$

Dislocations are assumed to be annealed and free to equilibrate. The Burgers vector charge density is an extra hydrodynamic variable with a conservation law,

$$\frac{\partial B_i}{\partial t} = -\partial_j J_j^i \; , \qquad (20)$$

where J_j^i is the Burgers current of the ith component of dislocation charge in the jth direction. For length scales longer than the average distance between free dislocations, $\xi_d \sim 1/\sqrt{n_f}$, and time scales longer than the mean collision time between free dislocations, one can make some simplifying approximations. Specifically, one can ignore the effect of dynamical polarization of bound dislocation pairs and also processes by which neutral dislocations pairs (i.e., dislocation pairs of opposite Burgers vectors) are created and annihilated. It was then shown in Ref. [12], that the constitutive relation for the Burgers current can be written as

$$J_j^i = -C_{jkl}^i(\sigma_{kl} + p_d\delta_{kl}) - D_{jl}^{ik}\partial_l B_k \; . \qquad (21)$$

The three terms on the right hand side of Eq. (21) correspond to the motion of dislocations in response to stresses in the lattice (the usual Peach-Koehler force), gradients in defect pressure and gradients in the dislocation density, respectively. The tensors C_{jkl}^i and D_{jl}^{ik} are given by

$$C_{jkl}^i = \frac{n_f a_0}{4k_B T}\left[(D_g - D_c)\delta_{jk}\epsilon_{li} + (D_g + 3D_c)\delta_{ik}\epsilon_{lj}\right] \; , \qquad (22a)$$

$$D_{jl}^{ik} = \frac{D_g - D_c}{4}(\delta_{ij}\delta_{kl} + \delta_{jk}\delta_{il}) + \frac{D_g + 3D_c}{4}\delta_{jl}\delta_{ik} \; , \qquad (22b)$$

where D_g and D_c are the diffusions constants for dislocation glide and climb, respectively.

The conservation laws for density and momentum, Eqs. (10a) and (10b), remain unchanged in the presence of dislocations. A new term must, however, be added to the equation for the conservation of defect density, reflecting the fact that a climbing dislocation acts as a source or sink of vacancies and interstitials. Equation (10c) is then replaced by

$$\frac{\partial n_\Delta}{\partial t} = -\nabla \cdot \mathbf{j}^\Delta + n_0 a_0 \epsilon_{ik} J_k^i \; . \qquad (23)$$

Since **u** is multi-valued, it is more convenient to consider an equation of motion for the strain rather than Eq. (10d) for the displacement field. This is given by

$$\frac{\partial w_{ij}}{\partial t} = \partial_i v_j - \frac{1}{n_0}\partial_i j_j^\Delta + a_0 \epsilon_{ik} J_k^j \; . \qquad (24)$$

where, to linear order, $\mathbf{g} = m n_0 \mathbf{v}$. The first two terms are simply obtained by differentiating the right hand side of Eq. (10d). The third term arises from the presence of dislocations.

The conservation laws of density, Eq. (10a), momentum density, Eq. (10b), defect density, Eq. (23), and Burgers vector charge, Eq. (20), together with the constitutive equations for the currents, Eqs. (11),(13) and (21), and the equation of motion for the local strains, Eq. (24), constitute a closed set of equations to describe the dynamics of a 2d solid with an equilibrium concentration of free annealed dislocations and of vacancy and interstitial defects.

The work by ZHN focused on the transverse and longitudinal hydrodynamic modes of these equations. These authors showed that the low frequency modes of a solid with dislocations are the same as those of the hexatic phase. In contrast, our goal here is to eliminate the dislocations and defects degrees of freedom and obtain a closed set of hydrodynamic equations for the density, momentum density and bond angle. By this procedure we show that the hydrodynamic equations of a solid with free dislocations are equivalent, at long wavelengths, to the hydrodynamic equations of a viscoelastic medium with bond angle order. The latter consists of conservation laws for the density and momentum density, an equation of motion for the bond angle, with a constitutive equation for the stress tensor that takes the form of a differential equation.

IV. HYDRODYNAMICS OF A VISCOELASTIC MEDIUM

Our strategy is to eliminate the defect density, n_Δ, and the Burgers-vector charge density, $\mathbf{B}$, from the hydrodynamic equations of a solid with dislocations discussed in the previous section. The outcome will be a closed set of equations for density, momentum density, bond angle field and stress tensor.

It is convenient to write the strain tensor w_{ij} as the sum of its symmetric and antisymmetric parts,

$$w_{ij} = (w_{ij} + w_{ji})/2 + (w_{ij} - w_{ji})/2$$
$$\equiv w_{ij}^s + w_{ij}^a . \qquad (25)$$

Only the symmetric part enters in the expression for the stress tensor, according to Eq. (13). One can therefore invert Eq. (13) to express w_{ij}^s as a function of the stress tensor and of the density, as

$$w_{ij}^s = \frac{1}{2\mu}\sigma_{ij} - \delta_{ij}\frac{\lambda+\gamma}{4\mu(\mu+\lambda+\gamma)}\sigma_{kk}$$
$$-\delta_{ij}\frac{\gamma}{2(\mu+\lambda+\gamma)}\frac{\delta n}{n_0} , \qquad (26)$$

where Eq. (17) was used to eliminate the defect density in favor of the density and the strain. The antisymmetric part, w_{ij}^a, has only one independent component which is simply the bond angle field, $\theta(\mathbf{r},t)$ [25],

$$w_{ij}^a = \epsilon_{ij}\theta . \qquad (27)$$

The equation of motion for the strain, Eq. (24), can then be split into an equation of motion for the symmetrized strain, given by

$$\frac{\partial w_{ij}^s}{\partial t} = v_{ij} - \frac{1}{2n_0}\Big(\partial_i j_j^\Delta + \partial_j j_i^\Delta\Big)$$
$$+\frac{a_0}{2}\Big(\epsilon_{ik}J_k^j + \epsilon_{jk}J_k^i\Big) , \qquad (28)$$

and an equation for the bond angle field,

$$\frac{\partial \theta}{\partial t} = \frac{1}{2}\hat{\mathbf{z}}\cdot(\nabla\times\mathbf{v}) - \frac{1}{2n_0}\epsilon_{ij}\partial_i j_j^\Delta + \frac{a_0}{2}J_k^k . \qquad (29)$$

We note that the trace of Eq. (28) simply gives the continuity equation for the density.

We can now use Eq. (26) to rewrite the equation of motion for the symmetric part of the strain tensor as a differential equation for the time evolution of the stress tensor, with the result

$$\frac{\partial \sigma_{ij}}{\partial t} = 2\mu v_{ij} + \lambda\delta_{ij}v_{kk}$$
$$+a_0\mu\Big(\epsilon_{ik}J_k^j + \epsilon_{jk}J_k^i\Big) + a_0(\lambda+\gamma)\delta_{ij}\epsilon_{kl}J_l^k$$
$$-\frac{\mu}{n_0}\Big(\partial_i j_j^\Delta + \partial_j j_i^\Delta\Big) - \frac{\lambda+\gamma}{n_0}\delta_{ij}\nabla\cdot\mathbf{j}^\Delta . \qquad (30)$$

In order to eliminate the defects and dislocation degrees of freedom, we now insert the constitutive equations for the defect and dislocation fluxes on the right hand side of Eqs. (29) and (30) and use $\delta n_\Delta = \delta n + n_0 w_{kk}^s$ and $B_j = \epsilon_{ik}\partial_i(w_{kj}^s + w_{kj}^a)/a_0$ to eliminate the defect density and dislocation density in favor of density and strain field. Finally, the strain field is related to the stress tensor and to the bond angle field using Eqs. (26) and (27). This completes the transformation of the equation for the strain tensor into two closed coupled equations for the stress tensor and the bond angle field.

For clarity, we present in this section the equations obtained when only terms of lowest order in the hydrodynamic fields are retained. In the next section we will include higher order terms and show that these yield wavevector dependent relaxation times for shear and compression. At long wavelengths, the gradients of the defect current density can be neglected both in the equation for the bond angle, Eq. (29), and in the equation for the stress tensor, Eq. (30). Similarly, one can drop the contribution to the dislocation current due to diffusion of dislocations and approximate

$$J_k^j \simeq -C_{knl}^j(\sigma_{nl} + p_d\delta_{nl}) \qquad (31)$$

or

$$J_k^j \simeq -C_{knl}^j\Bigg[\sigma_{nl} + \delta_{nl}\frac{\chi^{-1}+\gamma}{2(\mu+\lambda+\gamma)}\sigma_{kk},$$
$$-\delta_{nl}\frac{\chi^{-1}(\mu+\lambda)-\gamma^2}{\mu+\lambda+\gamma}\frac{\delta n}{n_0}\Bigg] . \qquad (32)$$

Carrying out some tedious algebra, we obtain the desired set of hydrodynamic equations, consisting of exact conservation laws for density and momentum, the equation for the bond angle field [26],

$$\frac{\partial \theta}{\partial t} = \frac{1}{2}\hat{\mathbf{z}}\cdot(\nabla\times\mathbf{v}) + \frac{D_g}{2}\nabla^2\theta , \qquad (33)$$

and the constitutive equation for the stress tensor,

$$\frac{\partial \sigma_{ij}}{\partial t} + \frac{1}{\tau_s}\tilde{\sigma}_{ij} + \frac{1}{2\tau_b}\delta_{ij}\sigma_{kk}$$
$$= 2\mu\tilde{v}_{ij} + B_\infty\delta_{ij}v_{kk} - \frac{B_0}{\tau_b}\delta_{ij}\frac{\delta n}{n_0} , \qquad (34)$$

where we recall that $B_\infty = \mu+\lambda$. The shear and compressional relaxation times (or "Maxwell" times) are given by

$$\frac{1}{\tau_s} = n_f\frac{D_g+D_c}{k_BT}\mu a_0^2 , \qquad (35)$$

$$\frac{1}{\tau_b} = n_f\frac{D_c}{k_BT}\frac{B_{eff}\chi^{-1}a_0^2}{B_0} , \qquad (36)$$

where $B_{eff} = \mu + \lambda - \chi\gamma^2$ is the "effective" bulk modulus that one would obtain by integrating out the defect density fluctuations from the free energy.
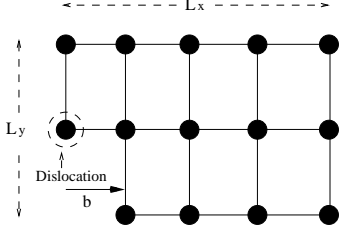
(a) The dislocation begins on the left side of the crystal, i.e. dx=0. The initial relative displacement of the upper and lower halves of the crystal is zero.
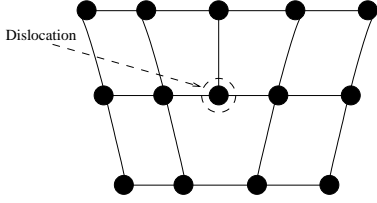
(b) The dislocation has glided two lattice spacings to the center of the crystal, i.e. dx=Lx/2. The relative displacement of the upper and lower halves of the crystal.
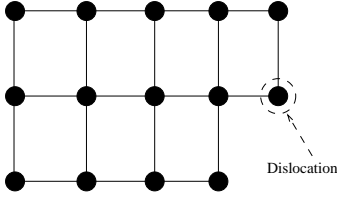
(c) The dislocation has now glided all the way to the right of the crystal, i.e. dx=Lx. The relative displacements of the upper and lower halves is now one lattice spacing.

FIG. 1. An illustration of how dislocation glide leads to relative displacement of two half crystals.

The shear relaxation time has a simple physical interpretation. Considering, for simplicity, only dislocation glide, the motion of a dislocation of Burgers vector $\mathbf{b} = \hat{\mathbf{x}}$ a distance dx along its slip line contributes an amount $\frac{a_0}{L_x}dx$ to the displacement of the half crystal, with L_x the length of the crystal along the slip direction. This is illustrated for a square lattice in Fig. (1). The corresponding change in shear strain is $\sim (a_0 dx/L_x)/L_y$, with L_y the width of the crystal in the direction normal to the slip line. The change in the strain γ in a time dt due to M dislocations is then $\frac{d\gamma}{dt} \simeq \frac{M}{L_x L_y} a_0 \frac{dx}{dt} = n_f a_0 v_g$, with $v_g = \frac{dx}{dt}$ the dislocation glide velocity. This is the well-known Orowan law [15] relating the plastic strain rate to the dislocation velocity. Dislocation motion is driven by local stresses and we can

write $v_g = \mu_g F_s$, with $\mu_g = D_g/(k_B T)$ the dislocation mobility and $F_s \approx \sigma_s a_0 \approx \mu a_0$ the force on a dislocation due to the shear stress, σ_s. If we define a shear relaxation time by $\frac{\gamma}{dt} \sim \frac{\gamma}{\tau_s}$, and assume $\gamma \sim \mathcal{O}(1)$, we immediately obtain $1/\tau_s \sim n_f \frac{D_g}{k_B T}\mu a_0^2$. When both glide and climb can occur the mobilities are simply additive.

An alternative interpretation of Eq. (35) is as follows. The rate at which dislocations diffuse thermally (via glide and climb) a distance of the order of the typical separation $\sim n_f^{-1/2}$ between free dislocations is $1/\tau_{th} = (D_g + D_c)n_f$. This is just the mean time for collisions between free dislocations. The ratio of the rate of diffusion of dislocations under the influence of shear elastic forces to the rate of thermal diffusion is of the order of the ratio of a typical shear elastic energy, μa_0^2 to thermal energy, $k_B T$. With this energetic argument we estimate $1/\tau_s \approx 1/\tau_{th}(\mu a_0^2/k_B T)$ which is the result given in Eq. (35). Interactions between dislocations are negligible only at time scales longer than the mean collision time, τ_{th} As a result our model applies only if $\tau_s > \tau_{th}$. Since $\mu a_0^2/k_B \sim \mathcal{O}(T_m)$, the condition $\tau_s > \tau_{th}$ simply corresponds to being above the melting temperature, T_m.

It is not surprising that the bulk memory time is independent of D_g, since pure compressional strains can only relax through dislocation climb. Also, since dislocation climb involves a change in particle number, D_c is, in general, much smaller than D_g, so that $\tau_s << \tau_b$. In addition, above the melting temperature the response to shear distortions is *purely* viscoelastic while the response to bulk distortions is effectively still elastic at large scales, with some dissipative effects (due to the climbing of dislocations) which, due to the smallness of D_c, are expected to be negligible.

In the limit of $n_f \to 0$, i.e., as T_m is approached from above, the shear and compressional relaxation times diverge, $\tau_{s,b} \to \infty$ according to Eq. (9), and we obtain

$$\frac{\partial \tilde{\sigma}_{ij}}{\partial t} = 2\mu \tilde{v}_{ij} , \tag{37a}$$

$$\frac{\partial \sigma_{kk}^{\text{dis}}}{\partial t} = 2(B_\infty - B_0)v_{kk} = -2\frac{B_\infty - B_0}{n_0}\frac{\partial \delta n}{\partial t} , \tag{37b}$$

In the absence of dislocations $v_{ij} = \partial_t w_{ij}^s$. Integrating Eq. (37a) then yields the shear stress-strain relation for an elastic solid,

$$\tilde{\sigma}_{ij} = 2\mu\left(w_{ij}^s - \frac{1}{2}\delta_{ij}w_{kk}^s\right) . \tag{38}$$

Similarly, to lowest order in the gradients, we can neglect the rate of change of defect density. Integrating Eq. (37b) and using Eq. (17), we then obtain $\sigma_{kk}^{\text{dis}} = (B_\infty - B_0)w_{kk}^s$ and

$$\sigma_{kk} = 2B_\infty w_{kk}^s . \tag{39}$$

Far above T_m, free dislocations proliferate and both τ_s and τ_b become very small. In this limit Eq.(34) then reduces to

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$$\sigma_{ij} = 2\mu\tau_s \tilde{v}_{ij} + \delta_{ij}(B_\infty - B_0)\tau_b \delta_{ij}\nabla \cdot \mathbf{v} - \delta_{ij}B_0\frac{\delta n}{n_0} \ . \quad (40)$$

Identifying the combinations $\mu\tau_s$ with the shear viscosity, η_s, and the combination $(B_\infty - B_0)\tau_b$ with the bulk viscosity, η_b, Eq. (40) is just the stress-rate of strain relation of a viscous liquid.

When only terms of lowest order in the gradients of the hydrodynamic fields are retained, it is not apparent from the viscoelastic stress-rate of strain relation that a crystal with annealed dislocations is a hexatic, rather than a isotropic viscous liquid. The presence of quasi-long-range bond orientational order in the hexatic manifests itself in a resistance to distortions that produce a non-zero gradient in the bond-angle field, θ. Contributions to the hydrodynamic equations from gradients of θ correspond to spatial gradients of w_{ij}, which have been neglected in this section. Such terms must be retained to see a signature of bond orientational order in the stress-rate of strain relations. This is done in the next section.

V. INCLUSION OF HIGHER ORDER GRADIENTS

In this section we incorporate all diffusive terms that were neglected in the previous section. We do so, however, only for a simplified model where dislocation climb is neglected. This corresponds to freezing out fluctuations in the defect density. It is an excellent approximation in most cases as the diffusion constant D_c for dislocation climb is generally very small due to the large energy cost of creating vacancies and interstitials. In the absence of fluctuations in the defect density the relation between symmetrized strain and stress simplifies to

$$w_{ij}^s = \frac{1}{2\mu}\sigma_{ij} - \frac{\lambda}{4\mu(\mu+\lambda)}\sigma_{kk}\delta_{ij} \ . \quad (41)$$

The exact conservation laws for density and momentum are of course unchanged and are still given by Eqs. (10a) and (10b), respectively. The equation of motion for the bond angle field now contains terms due to dislocation diffusion, which couple to gradients of stress and it is given by

$$\frac{\partial\theta}{\partial t} = \frac{1}{2}\hat{\mathbf{z}} \cdot (\nabla \times \mathbf{v}) + \frac{D_g}{2}\nabla^2\theta - \frac{D_g}{4\mu}\epsilon_{jk}\partial_i\partial_j\tilde{\sigma}_{ij} \ . \quad (42)$$

¿From Eq. (42), one sees that the presence of gliding dislocations leads to a dissipative term $\propto \nabla^2\theta$ and a coupling to $\tilde{\sigma}_{ij}$.

In the absence of fluctuations in the defect density, the stress tensor's trace is simply

$$\sigma_{kk} = -2B_\infty\frac{\delta n}{n_0} \ . \quad (43)$$

We therefore focus on its traceless part, $\tilde{\sigma}_{ij}$ Inclusion of the extra diffusive terms in the constitutive relation for $\tilde{\sigma}_{ij}$ will yield terms involving the gradient of the Burgers vector charge density. These terms are easily recast as gradients of bond angle and stress, resulting in the following constitutive relation for $\tilde{\sigma}_{ij}$

$$\frac{\partial\tilde{\sigma}_{ij}}{\partial t} + \frac{\tilde{\sigma}_{ij}}{\tau_s} - \frac{D_g}{4}\nabla^2\tilde{\sigma}_{ij}$$
$$= 2\mu\tilde{v}_{ij} + \frac{\mu D_g}{2}\left(\epsilon_{ik}\partial_j\partial_k + \epsilon_{jk}\partial_i\partial_k\right)\theta$$
$$+ \frac{\mu D_g}{4}\left(\partial_i\partial_j - \frac{\delta_{ij}}{2}\nabla^2\right)\frac{\delta n}{n_0} \ , \quad (44)$$

where Eq. (43) relating σ_{kk} and $\delta n/n_0$ has been used. It is instructive to rewrite Eq. (44) in Fourier space. The equation for $\tilde{\sigma}_{ij}(\mathbf{k}, t)$ is then given by

$$\frac{\partial\tilde{\sigma}_{ij}}{\partial t} + \frac{\tilde{\sigma}_{ij}}{\tau_s(k)} = 2\mu\tilde{v}_{ij} - \frac{\mu D_g}{2}\left(\epsilon_{ik}k_jk_k + \epsilon_{jk}k_ik_k\right)\theta$$
$$- \frac{\mu}{\tau_s(0)}\left(\hat{k}_i\hat{k}_j - \delta_{ij}/2\right)\xi^2k^2\frac{\delta n}{n_0} \ , \quad (45)$$

with $\hat{k}_i \equiv k_i/k$ and where we have defined

$$\xi \equiv \frac{1}{2}\sqrt{D_g\tau_s} \ . \quad (46)$$

One is naturally led to introduce a finite wavevector shear relaxation time, $\tau_s(k)$, given by

$$\tau_s(k) = \frac{\tau_s}{1+\xi^2k^2} \ . \quad (47)$$

When the constitutive relation is written in this form, it is apparent that ξ is the length scale beyond which the small gradient approximation is valid. At low frequency Eq. (45) reduces to

$$\tilde{\sigma}_{ij} = \frac{2\eta_s}{1+\xi^2k^2}\tilde{v}_{ij} - \frac{\mu D_g\tau_s(0)}{2(1+\xi^2k^2)}\left(\epsilon_{ik}k_jk_k + \epsilon_{jk}k_ik_k\right)\theta$$
$$- \frac{\mu}{1+\xi^2k^2}\left(\hat{k}_i\hat{k}_j - \delta_{ij}/2\right)\xi^2k^2\frac{\delta n}{n_0} \ . \quad (48)$$

By comparing Eq. (48) to the corresponding relation for a hexatic given in ZHN,

$$\tilde{\sigma}_{ij}^{hex} = 2\eta_s\tilde{v}_{ij} + \frac{K_A}{2}\left(\epsilon_{ik}\partial_j\partial_k + \epsilon_{jk}\partial_i\partial_k\right)\theta \ , \quad (49)$$

it is natural to identify the combination $\mu D_g\tau_s(0)$ with K_A, the elastic constant associated with long wavelength distortions of the bond angle field. The length scale ξ can then be written as

$$\xi \equiv \frac{1}{2}\sqrt{\frac{K_A}{\mu}} \quad (50)$$

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and it represents the length scale below which the energy associated with bond angle distortions becomes comparable to that associated with spatially uniform shear distortions.

The effective shear relaxation time, $\tau_s(k)$, is larger at short length scales, as the additional stiffness due to bond orientational order makes the system more solid-like. Finally, it should be noted that the term in Eq. (45) $\propto \delta n/n_0$ only contributes to the equation for the longitudinal ($\propto \nabla \cdot \mathbf{g}$) component of the momentum, but not to that for the transverse part ($\propto \nabla \times \mathbf{g}$). This indicates that, even if dislocation climb is forbidden, at short length scales the longitudinal component of momentum is affected by dislocation glide, which yields higher order pressure-like gradients in the equations of motion.

Clearly a regime where the wavevector dependence of the shear relaxation time is important only exists provided $\xi > \xi_d$, with $\xi_d \sim 1/\sqrt{n_f}$ the average distance between free dislocations. At length smaller than ξ_d interactions among dislocations can no longer be neglected and our model becomes invalid. It is easy to see that

$$\frac{\xi}{\xi_d} \sim \sqrt{\frac{k_B T}{\mu a_0^2}} \sim \sqrt{\frac{T}{T_M}} \ , \qquad (51)$$

with T_M the melting temperature of the two-dimensional lattice. Since our work always describes the region $T > T_M$, where free dislocations are present in the crystal, the wavevector dependence of the relaxation time will generally be important.

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[25] In a dislocation-free solid, the bond angle field is slaved to the displacement field and is given by $\theta = (\partial_x u_y - \partial_y u_x)/2$ In the presence of dislocations it can be rewritten as $\theta = \epsilon_{ij} w_{ij}/2$ which, when inverted, gives Eq. (27).

[26] The diffusive term in the equation for the time evolution of θ originates from the dislocation diffusion current that was neglected in the other equations. This term must, however, be incorporated in the equation for the bond angle field to obtain the lowest order term in the relaxation rate of the hexatic mode.