interface. The rational for interface dominated plasticity is simple: dislocations glide through the single crystal domain with relative ease, but pile up at interfaces, so that interface reactions become a critical step in continuing plastic deformation.

While the details of dislocation reactions at interfaces take place at the atomic scale, and the behavior of dislocations in bulk is most accurately modeled by discrete dislocation dynamics, both of these models are much too expensive and impractical for analyzing the resulting bulk behavior. The need for a continuum framework for describing the plasticity across crystal interfaces, including the ubiquitous size effects, is acute.

Recently developed size-dependent crystal plasticity theory employs the representation of the singular part of dislocation pile-up boundary layers as superdislocation boundary layers, or equivalently, as jumps in slip at the boundary, but internal to the crystal. These boundary superdislocations exist on two sides of an interface and react or combine to lower the total energy under certain conditions.

In this paper, we develop the continuum framework for interactions of dislocations at interfaces. The framework includes continuum kinematic description of dislocation reactions across an interface, geometrical and thermodynamic conditions for reactions, energy dissipation in interface reactions, as well as the kinetic barriers thresholds for the reactions.

We analyze the problem of single and double-slip shear of a thin film, and compare the results of continuum model with dislocation dynamics simulations.

Explicit forms of the entropy production and the degree of irreversibility for Navier-Stokes and Bingham fluids

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(joint work with B. Emek Abali)

1) The entropy inequality, normally known as the 2$^{\text{nd}}$ Law of Thermodynamics, is able to provide a measure of irreversibility. In here we consider an irreversible process, namely the flow of a non-linear viscous fluid in a two-dimensional channel, and use it in order to calculate the corresponding production of entropy as a function of classical material parameters, such as viscosity and heat conduction.
2) Thermodynamics of Irreversible Processes (T.I.P.) can be used to define a balance of entropy [1] with a strictly positive production term $\Sigma \geq 0$ by starting from the balance of internal energy (1$^{\text{st}}$ Law of Thermodynamics):

$$\rho \frac{\mathrm{d}u}{\mathrm{d}t} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ij} \frac{\partial v_i}{\partial x_j} \,, \tag{1}$$

employing the stress tensor in decomposed form $\sigma_{ij} = \frac{1}{3}\sigma_{kk}\delta_{ij} + \sigma_{\langle ij \rangle}$ and by assuming that the specific internal energy (per mass) $u = u(p, v)$ solely depends on the thermodynamical pressure p and the specific volume v, such that Eqn. (1) can be recast with the Gibbs' equation:

$$\frac{\mathrm{d}s}{\mathrm{d}t} = \frac{1}{T}\Big(\frac{\mathrm{d}u}{\mathrm{d}t} + p \frac{\mathrm{d}v}{\mathrm{d}t} \Big) \,, \tag{2}$$

into the balance of entropy:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V(t)} \rho s \,\mathrm{d}V = -\oint_{\partial V(t)} \frac{q_i}{T}\,\mathrm{d}a_i + \int_{V(t)} \Sigma \,\mathrm{d}V\,,$$

$$\Sigma = q_i \frac{\partial 1/T}{\partial x_i} + \sigma_{\langle ij\rangle}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + \frac{1}{T}\Big(\frac{1}{3}\sigma_{kk} + p\Big)\frac{\partial v_i}{\partial x_i}\,, \tag{3}$$

where absolute temperature $T > 0$ and mass density ρ are the primary variables and the heat flux q_i as well as the stress tensor σ_{ij} need to be specified in terms of those by constitutive relations. The first term on the right hand side may be interpreted as the flux of entropy across the boundaries of the thermodynamical system. Moreover the second term represents a production term, where the integrand Σ is always positive and reflects the 2^{nd} Law.

3) The constitutive relations must be in agreement with the latter condition. In order to see this more clearly, we rewrite the production term slightly:

$$\Sigma = -\frac{q_i}{T^2}\frac{\partial T}{\partial x_i} + \sigma_{\langle ij\rangle}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + \frac{1}{T}\Big(\frac{1}{3}\sigma_{kk} + p\Big)\frac{\partial v_i}{\partial x_i}\,. \tag{4}$$

It is now obvious that linear relations as proposed in [2], namely FOURIER's law $q_i = -\kappa\frac{\partial T}{\partial x_i}$ and $\sigma_{\langle ij\rangle} = \mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$ by putting $\kappa > 0, \mu > 0$ guarantee a non-negative production in case of an incompressible flow $\frac{\partial v_i}{\partial x_i}$. In particular we use for stress tensor a velocity dependent variable viscosity as in [3]:

$$\sigma_{ij} = -p\delta_{ij} + 2\mu(d_{(2)})d_{ij}\,,\ d_{ij} = \frac{\partial v_{(i}}{\partial x_{j)}}\,,\ d_{(2)} = \frac{1}{2}d_{ij}d_{ij}\,,$$

$$\mu = \mu_0 + \frac{1}{\pi}\frac{k}{\sqrt{d_{(2)}}}\arctan\Big(\frac{\sqrt{d_{(2)}}}{b}\Big)\,. \tag{5}$$

The three parameters μ_0, k, b are positive material constants. The first parameter μ_0 is the usual viscosity. If k vanishes the well-known NAVIER-STOKES relation for fluid matter results. Another limit case is obtained for vanishing b, so that the stress relation assumes a BINGHAM-type form. Then d_{ij}'s different from zero lead to an additional stress k, which can be interpreted in terms of a yield stress, known from solid matter. For this case it is even possible to find an analytical solution, which is briefly shown below.

4) Consider a two-dimensional finite channel filled with a viscous fluid, expressed in CARTESIAN coordinates with the horizontal x_1 and vertical x_2 axes. If the left and right ends of the channel experience a pressure gradient fluid motion will result. Also, if the top and bottom walls of the channel move at different speeds a velocity field in the fluid is created. We assume that both cases happen simultaneously and the flow process reaches a stationary state. If the fluid is pumped with a pressure gradient and sheared with moving walls, we assume that the motion occurs only in the horizontal direction depending on the height between the walls. This is generally the case for viscous fluids and can be represented by the semi-inverse ansatz $v_i = (v_1(x_2), 0)$. By using the aforementioned stress, heat flux relations for

the stationary case, the balance of momentum, introducing normalized quantities:

$$\bar{x} = \frac{x_2}{R}\,,\ \bar{v} = \frac{v_1}{v_0}\,,\ v_0 = \frac{|p'|R^2}{\mu_0}\,,\ \bar{\sigma} = \bar{v}' \mp \bar{k}\,,\ \bar{k} = \frac{k}{|p'|R}\,,\ \bar{\sigma}_{ij} = \frac{\sigma_{21}}{|p'|R}\,, \tag{6}$$

the velocity field reads:

$$\bar{v}(\bar{x}) = \begin{cases} \frac{1}{2}\left(1-\bar{x}^2\right) - \xi\,(1+\eta)\,(1-\bar{x}) + v_{\text{top}} & , \quad \forall \bar{x} : \xi + \eta\xi \le \bar{x} \le 1 \\ \text{const.} & , \quad \forall \bar{x} : -\xi + \eta\xi \le \bar{x} \le \xi + \eta\xi \\ \frac{1}{2}\left(1-\bar{x}^2\right) - \xi\,(1-\eta)\,(1+\bar{x}) + v_{\text{bottom}} & , \quad \forall \bar{x} : -1 \le \bar{x} \le -\xi + \eta\xi. \end{cases} \tag{7}$$

From the balance of internal energy:

$$-\kappa \frac{\mathrm{d}^2 T}{\mathrm{d}x_2^2} = \sigma_{21} \frac{\mathrm{d}v_1}{\mathrm{d}x_2}\,,\ \bar{T} = \frac{T}{T_0}\,,\ \bar{p} = \frac{|p'|R}{k}\,,\ \bar{\kappa} = \frac{\kappa T_0}{k v_0 R}\,,$$

$$\bar{T} = \frac{\bar{p}}{12\bar{\kappa}}\left(1 - \bar{x}^4 - 2(\bar{x}^3 \pm 1)\alpha + 6(\bar{x}^2+1)\beta\right) + c(\bar{x} \mp 1) + 1\,, \tag{8}$$

$$\alpha = 2\eta\xi \pm 2\xi \mp \bar{k}\,,\ \beta = \xi^2(1+\eta^2) \pm 2\eta\xi^2 - \bar{k}\xi(1 \pm \eta)\,, \tag{9}$$

we obtain a temperature distribution for the case of identical temperatures at the boundaries $T|_{\pm 1} = T_0$, identical heat fluxes in the transition points $\bar{\kappa}\frac{\mathrm{d}\bar{T}}{\mathrm{d}\bar{x}}|_{\xi\eta+\xi} = \bar{\kappa}\frac{\mathrm{d}\bar{T}}{\mathrm{d}\bar{x}}|_{\xi\eta-\xi} = \bar{\kappa}c$, and the same thermal conductivities in both regimes. Finally we obtain for the entropy production or rather for the dissipation function Φ mentioned in [3]:

$$\Sigma = \frac{\kappa}{T^2}\left(\frac{\mathrm{d}T}{\mathrm{d}x_2}\right)^2 + \frac{1}{T}\sigma_{21}\frac{\mathrm{d}v_1}{\mathrm{d}x_2}\,,\ \bar{\Sigma} = \frac{T_0 R}{k v_0}\Sigma \tag{10}$$

$$\Phi = \bar{T}\bar{\Sigma} = \frac{\bar{\kappa}}{\bar{T}}\left(\frac{\mathrm{d}\bar{T}}{\mathrm{d}\bar{x}}\right)^2 + \frac{1}{\bar{k}}\left(\frac{\mathrm{d}\bar{v}}{\mathrm{d}\bar{x}}\right)^2 \mp \frac{\mathrm{d}\bar{v}}{\mathrm{d}\bar{x}}\,. \tag{11}$$

This function can be considered as a measure of irreversibility. It consists of two coupled parts, a mechanical and a thermal one. Although we start with a mechanically driven system, the calculation shows that the induced temperature field adds an important amount to the dissipation function. Hence, as the dissipation function with its mechanical and thermal parts for a flow with velocity field can be seen in Fig. 1, even in a purely mechanically driven viscous flow, one shall not neglect the thermal dissipation out of the system.

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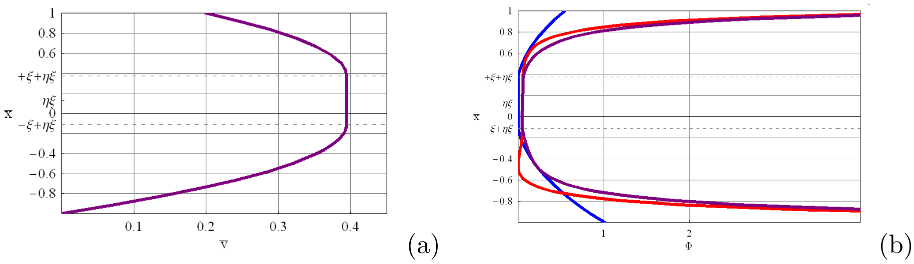

FIGURE 1. (a) Velocity profile, (b) Dissipation function (purple) with its mechanical (red) and thermal (blue) parts.

Material instability: Implications for extracting material response from specimen measurements

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(joint work with Shelby B. Hutchens, Nisha Mohan, Julia R.Greer)

Vertically aligned carbon nanotubes (VACNTs) have shown promising mechanical properties for use in a variety of applications, for example, energy absorption, compliant thermal interfaces and biomimetic dry adhesives. In some cases VACNTs have displayed high recoverability after significant strain while other in other cases permanent deformations have been observed. In particular, Hutchens et al. [1] have observed large permanent deformations in compression of micron scale pillars that deform by progressive buckling. The relative density of the pillars (pillar density/fully dense material) is about 13% so these materials are highly compressible. The overall response that is obtained from such a test is a "structural" response in that the response depends on the pillar geometry and the loading (and support) conditions. One would like to be able to extract a material property from this response where by a material property is meant a parameter value or a function that can be used to predict the response of the material under other loading conditions. Of course, what constitutes a property depends on the constitutive theory used to describe the material response.

Calculations in [2] showed that a simple rate dependent elastic-viscoplastic constitutive relation with a hardening-softening-hardening form of the flow strength as a function of plastic strain that also accounted for plastic compressibility could at qualitatively, and in some aspects quantitatively, represent the main observed features. A microstructurally motivation for this constitutive description is given in [3].

The analyses in [2] raise the question of how to extract material properties from tests on materials exhibiting this type of constitutive response. To explore this we consider the response of a compressible elastic-viscoplastic solid with the four flow strength relations shown in Fig. 1 subject to: (i) uniaxial tension, (ii) uniaxial compression and (iii) indentation with a sharp indenter. Material A, which exhibits softening, is representative of the flow strength description used in [2].