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Relations between material mechanical parameters and interparticle potential in amorphous solids

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The shear modulus and yield stress of amorphous solids are important material parameters, with the former determining the rate of increase in stress under external strain and the latter being the stress value at which the material flows in a plastic manner. It is therefore important to understand how these parameters can be related to the interparticle potential. Here a scaling theory is presented such that given the interparticle potential, the dependence of the yield stress, and the shear modulus on the density of the solid can be predicted in the athermal limit. It is explained when such prediction is possible at all densities and when it is only applicable at high densities.

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I. INTRODUCTION

Typical solids, whether amorphous or crystalline, respond linearly and elastically to small strains. Then the stress $\sigma_{\alpha\beta}$ increases like $2\mu\epsilon_{\alpha\beta}$, where μ is the shear modulus, $\epsilon_{\alpha\beta}$ is the strain,

$$\epsilon_{\alpha\beta} \equiv \frac{1}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right), \tag{1}$$

and $\boldsymbol{u}$ is the displacement field. Upon increasing the strain further, the material yields and begins to flow; the average stress value in the plastic steady state is defined here as the "yield stress" σ_Y. In crystalline materials this plastic flow is understood in terms of the motion of defects such as dislocations.[1] It is much less clear in amorphous solids what the carriers of plasticity are and how to relate the onset of plasticity to the microscopic properties of the material. The aim of this Rapid Communication is to present a scaling theory that is able, subject to stated conditions, to predict how μ and σ_Y depend, say, on the density of the material. In addition we clarify the issue of universality of the ratio μ/σ_Y which had come up in recent experiments on a family of metallic glasses.[2]

II. YIELDS STRESS AND THE ENERGY DROPS

To initiate the discussion we remind the readers of a typical strain-stress curve in amorphous materials. For this purpose we construct a glassy system consisting of polydispersed soft disks. We work with N point particles of equal mass m in two dimensions with pairwise interaction potentials. Each particle i is assigned an interaction parameter λ_i from a normal distribution with mean $\langle\lambda\rangle = 1$. The variance is governed by the polydispersity parameter $\Delta = 15\%$, where $\Delta^2 = \frac{\langle(\lambda_i - \langle\lambda\rangle)^2\rangle}{\langle\lambda\rangle^2}$. With the definition $\lambda_{ij} = \frac{1}{2}(\lambda_i + \lambda_j)$, the potential is constructed such as to minimize computation time,[3]

$$U(r_{ij}) = \begin{cases} \epsilon\left[\left(\frac{\lambda_{ij}}{r_{ij}}\right)^k - \frac{k(k+2)}{8}\left(\frac{B_0}{k}\right)^{(k+4)/(k+2)}\left(\frac{r_{ij}}{\lambda_{ij}}\right)^4 + \frac{B_0(k+4)}{4}\left(\frac{r_{ij}}{\lambda_{ij}}\right)^2 - \frac{(k+2)(k+4)}{8}\left(\frac{B_0}{k}\right)^{k/(k+2)}\right], & r_{ij} \le \lambda_{ij}\left(\frac{k}{B_0}\right)^{1/(k+2)} \\ 0, & r_{ij} > \lambda_{ij}\left(\frac{k}{B_0}\right)^{1/(k+2)}, \end{cases} \tag{2}$$

where r_{ij} is the separation between particles i and j. The shape of this potential for $k=8$ and $k=10$ is shown in Fig. 1. Below the units of length, energy, mass, and temperature are $\langle\lambda\rangle$, ϵ, m, and ϵ/k_B, where k_B is the Boltzmann constant. The unit of time τ_0 is accordingly $\tau_0 = \sqrt{(m\langle\lambda\rangle^2/\epsilon)}$. In the present simulations we choose $B_0 = 0.2$ and employ an athermal quasistatic scheme[3] with Lees-Edwards boundary conditions. After each strain step energy minimization was carried out until $|\nabla U|^2/N \le 10^{-18}$. Initial conditions were prepared by instantaneously quenching random configurations. In Fig. 2 we show a typical stress-strain curve for this model with $N=4096$ and $k=10$. For small strains the stress grows linearly with a slope μ; this continues as long as the material is elastic, i.e., for stress less than σ_Y. For stress that exceeds σ_Y,

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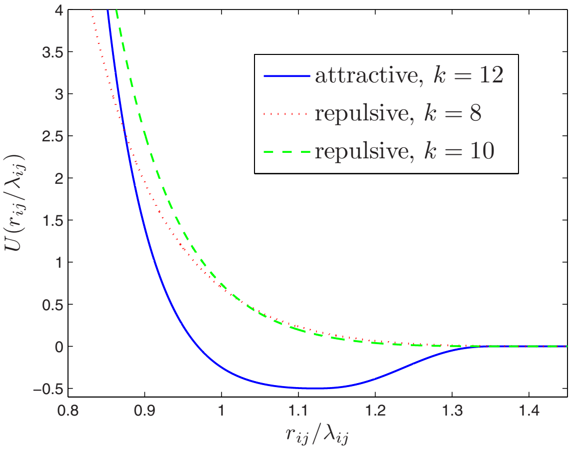

FIG. 1. (Color online) The three different pairwise potentials discussed in this Rapid Communication.

plastic events begin to take place. In this regime we observe drops in the stress of size Δ_σ, and we denote the mean size of these stress drops by $\langle\Delta_\sigma\rangle$. Between the stress drops the strain is increased by intervals Δ_ϵ with a mean $\langle\Delta_\epsilon\rangle$. Associated with the stress drops are potential-energy drops which we denote by Δ_U whose mean is $\langle\Delta_U\rangle$. In Ref. 3 the dependence of these averages on the system size was determined, with the results

$$\langle\Delta_\sigma\rangle = C_\sigma N^\beta, \quad \langle\Delta_U\rangle = C_U N^\alpha, \tag{3}$$

with C_σ having the units of stress and C_U of energy. The exponents satisfy a scaling relation $\alpha-\beta=1$ which can be easily derived from the exact energy conservation relation[3,4] in the elastoplastic steady state where the mechanical properties reach a saturated value,

$$\sigma_Y\langle\Delta_\epsilon\rangle V = \sigma_Y\frac{\langle\Delta_\sigma\rangle}{\mu}V = \langle\Delta_U\rangle. \tag{4}$$

Substituting Eq. (3) into Eq. (4), the experimental fact that σ_Y and μ are intensive quantities independent of N implies $\alpha-\beta=1$, and we can rewrite the last equation in favor of the yield stress σ_Y,

$$\sigma_Y = \frac{\rho C_U\mu}{C_\sigma}, \tag{5}$$

where $\rho \equiv N/V$ is the number density. Note that the combination $\Omega^{-1} \equiv \rho C_U/C_\sigma$ is a pure number whose nonuniversality will be discussed below. The challenge at this point is to provide a theory for the dependence of μ and the prefactors C_σ and C_U on the experimental control parameters. In this Rapid Communication we focus on the athermal limit $T=0$ and study the density dependence; the thermal theory is more involved and will be dealt with in a future publication.

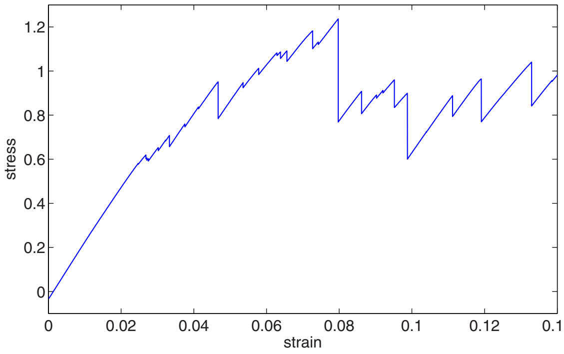

FIG. 2. (Color online) Typical stress-strain curve for a system with $N=4096$ and $k=10$ in Eq. (2).

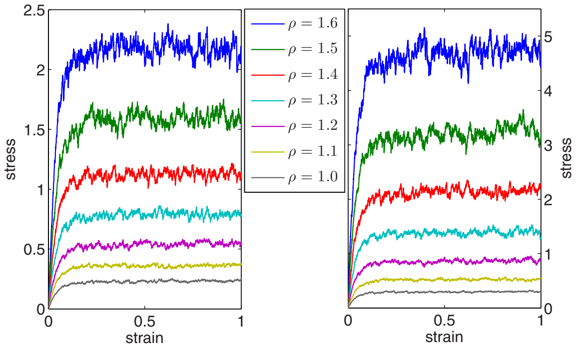

FIG. 3. (Color online) Stress-strain curves averaged over 20 independent runs for an athermal system with $N=4096$, $k=8$ (left panel), and $k=10$ (right panel) as a function of the density, with the density increasing from bottom to top.

III. RESULTS AND SCALING THEORY

In Fig. 3 we present the stress-strain curves of two systems, each with $N=4096$, as a function of the density, one with $k=8$ in Eq. (2) and one with $k=10$. We note the very strong dependence of both μ and σ_Y on the density (60% change in the density results in a factor of up to 20 in σ_Y). We also note the sensitivity to the repulsive law of the potential, changing k by 25% changes the yield stress by a factor of 2. To understand this density dependence we point out that both σ_Y and μ have the dimensions of stress, and from the potential the quantity having the same dimension is the function $r^{-1}\frac{\partial U(r)}{\partial r}$. Thus if this function has a scaling behavior with r then σ_Y and μ would have a related scaling behavior with ρ. If $U(r)$ were a simple power law r^{-k}, this function would behave like r^{-k-2} or scale with ρ as $\rho^{(k+2)/2}$ since $\rho \sim r^{-2}$. Potential (2) is not a simple power law but as we shall see the function $r^{-1}\frac{\partial U(r)}{\partial r}$ exhibits an effective power law or scaling behavior. We compute $r^{-1}\frac{\partial U(r)}{\partial r}$ in the range of $r \in [\rho_{\max}^{-1/2}, \rho_{\min}^{-1/2}]$ (see Fig. 4).

We find that to a very good approximation

$$\frac{1}{r}\frac{\partial U(r)}{\partial r} \sim r^{-2\nu}, \tag{6}$$

with $\nu=4.80$ for $k=8$ and $\nu=5.87$ for $k=10$. With this effective scaling behavior, we can predict *a priori* that Ω^{-1}, being a number, should be independent of ρ and both σ_Y and $\langle\mu\rangle$ should scale like

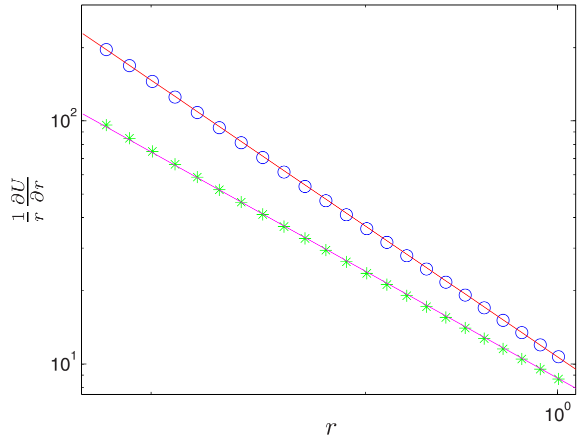

FIG. 4. (Color online) $r^{-1}\frac{\partial U(r)}{\partial r}$ in the range of $r \in [\rho_{\max}^{-1/2}, \rho_{\min}^{-1/2}]$. The line through the points represents the scaling laws (6).

$$\sigma_Y \sim \rho^{\nu}, \quad \langle \mu \rangle \sim \rho^{\nu}, \tag{7}$$

where $\langle \mu \rangle$ denotes an average of the shear modulus over the elastic steps of the steady-state plastic flow. Consequently we expect that the stress-strain curves would collapse by dividing all the stresses by ρ^{ν}. Figure 5 demonstrates the perfect data collapse under this rescaling, together with the high precision of the scaling laws (7).

IV. WHEN SCALING FAILS

To delineate the applicability of the scaling theory, we turn now to a third potential in which to the repulsive branch we add an attractive one (see Fig. 1). The potential chosen reads (with the same polydispersity of λ_{ij})

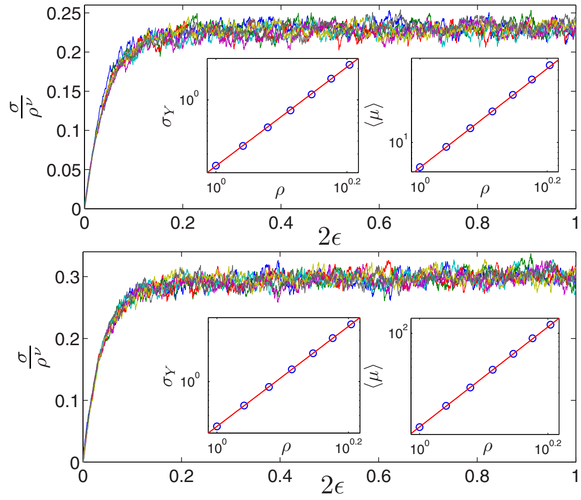

FIG. 5. (Color online) The same stress-strain curves as in Fig. 3 but with the stress rescaled by ρ^{ν}, with $\nu=4.80$ for $k=8$ (upper panel) and $\nu=5.87$ for $k=10$ (lower panel). The insets demonstrate the density dependence of σ_Y and μ according to ρ^{ν}.

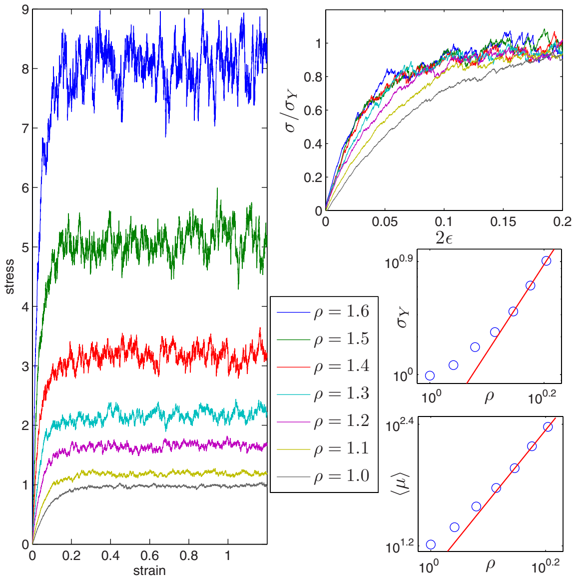

FIG. 6. (Color online) Left panel: stress-strain curves for potential (8) which has repulsive and attractive parts. Right upper panel: demonstration of the failure of rescaling of the stress-strain curves. Lower panels: σ_Y and $\langle \mu \rangle$ as functions of the density. Note that predictability is regained only for higher densities, the straight line is ρ^7.

$$U(r) = \begin{cases} \tilde{U}(r_{ij}), & r \le r_0(\lambda_{ij}) \\ \hat{U}(r_{ij}), & r_0(\lambda_{ij}) < r \le r_c(\lambda_{ij}) \\ 0, & r > r_c(\lambda_{ij}), \end{cases} \tag{8}$$

with $\tilde{U}(r_{ij}) = \epsilon[(\frac{\lambda_{ij}}{r_{ij}})^k - (\frac{\lambda_{ij}}{r_{ij}})^6 - 1/4]$; $k=12$, $r_0=2^{1/6}\lambda_{ij}$, and $r_c=1.36\lambda_{ij}$. The attractive part $\hat{U}(r)$ is glued smoothly to the repulsive part. We choose $\hat{U}(r)=\frac{\epsilon}{2}P(\frac{r-r_0}{r_c-r_0})$, where $P(x)=\Sigma_{i=0}^{5}A_i x^i$ and the coefficients A_i are chosen such that the potential is smooth up to second derivative.[5] We repeated the measurements of the stress-strain curves for this system, now with $N=2500$, and displayed the results in Fig. 6, left panel. In the right upper panel we show what happens when we try to collapse the data by rescaling the stress by σ_Y. Of course the stress-stain curves now all asymptote to the same value, but the curves fail to collapse, since μ does not in general scale in the same way as σ_Y. The reason is the failing of the scaling hypothesis in this case: the calculation of $r^{-1}\frac{\partial U(r)}{\partial r}$ in the range of $r \in [\rho_{\max}^{-1/2}, \rho_{\min}^{-1/2}]$ fails to provide an effective power law, destroying the scaling hypothesis and the data collapse. Nevertheless even in the present case we can have predictive power for high densities. When the density increases the repulsive part of potential (8) becomes increasingly more relevant, and the inner power law r^{-12} becomes dominant. We therefore expect that for higher densities scaling will be regained, and both σ_Y and $\langle \mu \rangle$ would depend on the density as ρ^7. The two lower right panels in Fig. 6 show how well this prediction is realized also in the present case.

We therefore conclude that given a potential one should be able to decide whether a scaling theory should be appli-

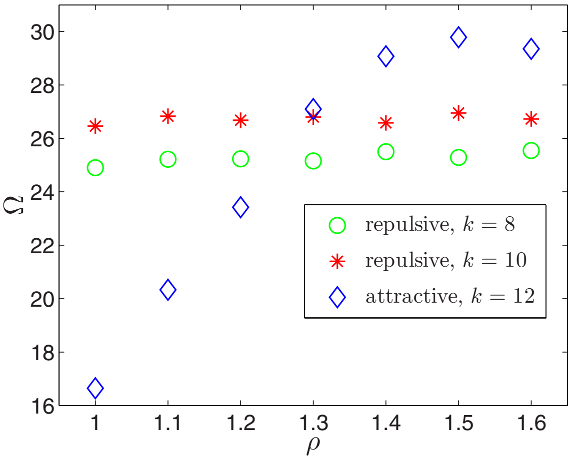

FIG. 7. (Color online) The pure number Ω as a function of the density for the three potentials discussed in the text. Note that Ω appears to increase with the exponent of the repulsive part of the potential whenever scaling prevails.

cable and at what densities. Whenever the most probable interparticle distance agrees with the average interparticle distance, scaling can be employed with impunity. At low densities this condition may not apply due to the attractive part of the potential. Nevertheless with higher densities scaling and predictability of the mechanical properties should get better and better.

Finally we discuss the numerical value of the parameter $\Omega = C_\sigma / (\rho C_U)$. We note that the data collapse indicates that this parameter is, to a very good approximation, independent of ρ for a given potential function. For the two different potentials (2) with $k=8$ and $k=10$, respectively, we find from our numerics that this parameter differs by about 5%, indicating nonuniversality. The lack of universality is even clearer with the last potential (8). In Fig. 7 we display the computed values of Ω for the three cases studied above. When scaling prevails the value of Ω is constant up to numerical fluctuations. In the third case, where scaling fails, Ω is a strong function of ρ except at higher densities where scaling behavior is recaptured as explained. We can therefore conclude that the approximate constancy of Ω found in a family of metallic glasses[2] is not fundamental but only an indication of the similarity of the potentials for this family. In general Ω can depend on the interparticle potential. It is quite clear from considering Eqs. (6) and (7) that the *coefficients* in the scaling laws (7) may well depend on the exponent k in the repulsive part of the potential. The ratio of these prefactors, being a pure number, could be independent of k, and Ω could be universal. It appears however that μ is increasing more with k than σ_Y, and Ω shows a clear increase upon increasing k. At present this must remain an interesting riddle for future research.

In summary, we have begun in this Rapid Communication to explore the relations between interparticle potentials and the mechanical properties of amorphous solids that are made of these particles. We note that similar considerations were presented for the dynamics of supercooled liquids, first experimentally[6] and then theoretically.[7] Presently we focused on the athermal limit and showed how the dependence of the yield stress and the shear modulus on the density can be determined from first principles as long as the scaling hypothesis prevails. We also examined when this hypothesis failed and pointed out that in any material the theoretically determined relations can be trusted at high densities. It is interesting to note that for supercooled liquids the existence of attractive branches in the pairwise potential appears less destructive for a scaling theory. In later publications we will examine the effect of temperature and strain rate on the present issues.

ACKNOWLEDGMENTS

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