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Internal, elastic stresses below randomly rough contacts

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ABSTRACT

Knowing the stress tensor inside a body is central to predict the onset of plastic deformation in an initially elastic solid that is squeezed against a rigid counterface. However, recent studies of mechanical contacts between randomly rough solids only elucidated the distribution functions and spatial correlations of the normal stress within the interface. This work reveals that typical normal and von Mises stresses, the latter being central to classical plasticity theory, take their maxima at or near the interface below patches of true contact and then decay quite slowly with increasing depth. They only level off at a depth that roughly equals the in-plane distance at which the height-difference auto-correlation function saturates. The results are rationalized with an extension of Persson theory to internal stresses. The central quantity arising from this extension is a depth-dependent, root-mean-square height gradient, in which short-wavelength surface ondulations are damped out. It allows quick estimates to be made of characteristic, internal peak stresses within mechanically loaded solids having randomly rough surfaces.

1. Introduction

When two nominally flat solids touch, true contact only tends to be made at a small fraction of the apparent contact area, because even highly polished surfaces maintain non-negligible roughness at small scales (Bowden and Tabor, 1986; Whitehouse and Archard, 1970). Load is predominantly carried by the tops of a few peaks, where stresses are consequently large, while no external stress acts on deep valleys. Due to the self-affine nature of many natural and technological surface topographies (Majumdar and Tien, 1990; Palasantzas, 1993; Persson, 2014), a complex contact geometry arises, which turns a reliable prediction of contact stresses into a challenging exercise (Carpick, 2018; Müser et al., 2017).

It is now agreed upon that typical, local normal stresses at the interface between two nominally flat, elastic solids are of the order of the contact modulus E^* (defined further below) times the root-mean square (rms) height gradient $\bar{g}$ (Campañá and Müser, 2007; Hyun et al., 2004; Persson, 2001; Prodanov et al., 2013; Putignano et al., 2012; Yastrebov et al., 2015). The latter is a scale-dependent quantity; the larger the resolution, the finer the features that can be perceived (Persson, 2001; 2006). This is why measurements of not only $\bar{g}$ but also of other properties, such as the relative contact area a_r, turn out to be functions of the smallest in-plane distance Δr that can be resolved. For a given height spectrum, this insight immediately allows a rough estimate to be made on how quickly the normal stress decreases on average with the lateral distance Δr from a point of contact. Accurate scaling laws including prefactors can be obtained either with Persson theory (Persson, 2008; Wang and Müser, 2018) or from rigorous contact-mechanics simulations (Campañá et al., 2008; Wang and Müser, 2018).

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While normal surface stresses are certainly interesting to know, successful criteria for the onset of plasticity cannot be based on a single stress-tensor element, because plastic flow is usually triggered by the anisotropy of stress. A measure for the anisotropy of stress is the von Mises stress $\sigma_{\rm v}$, defined as 1.5 times the standard deviation of the principal stresses. The most popular, macroscopic yield criterion, applied predominantly to isotropic, ductile materials, requires the von Mises stress to remain below the yield strength (von Mises, 1913). So far little is known about the statistical properties of von Mises stresses in randomly rough contacts. Persson theory and most large-scale simulations of solids with random roughness have been predominantly concerned with interfacial, normal stresses. While the pioneering simulations by Pei et al. (2005) considered J2 plasticity in the bulk, the focus was laid on the question how plasticity affects the shape and the magnitude of the true contact area. In contrast, this work is concerned with a systematic analysis of how local stresses decrease on average with depth below contact patches. Towards this end, simulations and Persson theory address various statistical properties of normal and von Mises stresses.

The simulations and theory presented in this work consider a frictionless contact between a rough, rigid indenter and a flat, elastic solid. However, the small-slope approximation (Johnson, 1985) makes it possible to relate the results to other systems, in which surface roughness and elastic compliance are divided up more evenly between the two counterfaces. The surface roughness is designed to mimic typical surface topographies. It contains a self-affine scaling regime, in which the expected height variance averaged over circles of radius r increases as r^{2H} (Schmittbuhl et al., 1995), where H is the Hurst roughness exponent, plus a roll-off domain, in which the height variance no longer varies noticeably once r exceeds the roll-off wavelength $\lambda_{\rm r}$. The usual linear relations between surface displacement and surface stress are assumed. Stress-tensor components decay essentially exponentially with depth at a rate proportional to the wave vector of a height undulation. Simulations are run with the Green's function molecular dynamics (GFMD) technique (Campañá and Müser, 2006). Details of the model and the simulations are summarized in the methods section, along with a derivation and discussion of an integral transform relating the in-plane (normal) stress autocorrelation function (ACF) to other stress ACFs. The extension of Persson theory to internal stresses is developed in the results section. The fundamental idea behind the extension is that stress "smears out" with increasing depth in a similar way as with decreasing resolution. Technically, this can be described with an effective, depth-dependent rms height gradient, which allows results obtained for interfacial stresses to be ported to internal stresses.

2. Model and methods

The studied system is an "*in-silico* contact" composed of a rough, rigid indenter fixed in space and a semi-infinite, elastic half space to which a constant external pressure is applied squeezing it against the indenter. The interaction between the two bodies is a non-overlap constraint.

The surface topography of the indenter and the elastic properties of the half space are defined further below in this section. In addition, the employed numerical technique (GFMD) shall be sketched along with some mathematical calculations, which are predominantly technical in nature but useful for the analysis and interpretation of the results. This includes the derivation of two integral transforms for stress ACFs, which may be interesting in their own right.

2.1. System geometry

The mean surface normal of the interface is parallel to the z-axis. Periodic boundary conditions are applied in the xy-plane to reduce finite-size effects. The indenter is assigned a height topography $h(\mathbf{r})$, where $\mathbf{r} = (x, y)$ is a vector within the interfacial plane. $h(\mathbf{r})$ is generated assuming the random-phase approximation for the Fourier coefficients $\tilde{h}(\mathbf{q})$, i.e., $\tilde{h}(\mathbf{q}) \propto \sqrt{C(\mathbf{q})}\exp(i2\pi\zeta_{\mathbf{q}})$, where $\zeta_{\mathbf{q}}$ is an independent random variable uniformly distributed on (0,1). The proportionality constant is chosen such that the $\bar{g} = 1$ at infinite resolution. The used height spectrum reads

$$C(q) = \frac{C_0 \cdot \Theta(q_{\rm s} - q)}{\{1 + (q/q_{\rm r})^2\}^{1+H}}, \tag{1}$$

where H is the Hurst roughness exponent and $\Theta(\bullet)$ the Heavyside step function. $q_{\rm r} = 2\pi/\lambda_{\rm r}$ and $q_{\rm s} = 2\pi/\lambda_{\rm s}$ are the wave numbers associated with the roll-off and short wavelength cutoff, respectively. The smooth transition from the self-affine domain, where $C(q) \approx C_0(q/q_{\rm r})^{2(1+H)}$, and the roll-off domain, where $C(q) \approx C_0$, was chosen, because this represents experimental data better than a sharp transition (Majumdar and Tien, 1990; Palasantzas, 1993; Persson, 2014). Moreover, ringing effects in real-space stress-ACFs are reduced with a smooth transition.

The default system has a linear size of $L = 4\lambda_{\rm r}$ with $\lambda_{\rm r} = 2\pi/q_{\rm r}$ and a roll-off wavelength of $512\lambda_{\rm s}$. Depending on the quantity of interest, different choices for the spectrum were occasionally made. For example, to obtain statistically relevant data for the stress distribution function at a depth of $z = 50\lambda_{\rm s}$ from GFMD, the simulated system was assigned a system size of 8 $\lambda_{\rm r}$ (to improve statistics) and the grid spacing increased to $2\lambda_{\rm s}$ (to save computer time).

The height spectrum and the square root of the height-difference ACF $G_{\delta h}(\Delta r)$ pertaining to the default system are shown in Fig. 1. The height difference ACF,

$$G_{\delta h}(\Delta r) \equiv \left\langle \{h(\mathbf{r}) - h(\mathbf{r} + \Delta\mathbf{r})\}^2 \right\rangle \big/ 2 \tag{2}$$

allows several central quantities to be readily determined (Wang and Müser, 2018). For example, the height variance corresponds to $G_{\delta h}(\Delta r \to \infty)$, while $\bar{g}(0)$ at infinite resolution equals $2\sqrt{G(\Delta r)}/\Delta r$ in the limit of $\Delta r \to 0$.