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Present and future of atomistic simulations of dislocation plasticity

Commentary by

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on

Atomistic insights into metal hardening
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Statement of Significance

Zepeda-Ruiz et al. [1] is a landmark paper showing what ultra-large-scale atomistic simulations can teach us about plastic deformation of metallic single crystals. In particular, this work presents the currently least-biased predictions of strain hardening caused by dislocation interactions. The generated data is likely to become a major reference for the development or refinement of hardening laws used in models at larger size scales, such as discrete dislocation plasticity and crystal plasticity.

Position in the field of multiscale plasticity

In the common view of scale bridging in multiscale plasticity of crystalline metals, classical molecular dynamics (MD) is followed by discrete dislocation plasticity (DDP) and subsequently by crystal plasticity (CP). These three approaches describe emergent behaviour: (i) in MD, the classical motion of the nuclei is retained while the electronic degrees of freedom are coarse-grained to an empirical potential that mimics the interatomic forces; (ii) in DDP the atoms are coarse-grained out to an elastic continuum while the dislocations are retained as borders of patches with slip discontinuities; (iii) subsequently, in CP the motion of dislocations is further coarse-grained to a field of slip rates on distinct slip systems.

Every scale bridging step reduces the number of degrees of freedom, which allows for the description of plasticity at increasingly larger length and time scales. Keeping in mind that $1\ \mu\text{m}^3$ of an FCC crystal contains on the order of 10^{11} atoms, it is obvious that even the ultra-large-scale MD simulations in [1] cannot be adopted directly in micron-scale applications. At those length scales, DDP can be a powerful tool, while CP becomes convenient to describe plasticity at even larger length scales. Moreover, coarse-graining in length scale implies scale bridging in time, allowing simulation times beyond the hundreds of nanoseconds achieved in [1]. The work by Zepeda-Ruiz et al. [1] provides a wealth of computational data aiming to bridge the scale from MD to CP, in particular regarding hardening. We will argue below that these findings also contain relevant information to enrich constitutive models in DDP. Yet, we will proceed by first reminding the reader of the limitations of these atomistic studies.

Limitations of atomistics for plasticity

It is well known that embedded atom method (EAM) interatomic potentials for MD simulations, like the one used in [1], can suffer from artifacts when applied to simulate atomic environments that are not directly linked to the properties they have been fitted to. Predictive capabilities of MD simulations might be limited because of (i) the absence of accurate phonon spectra [2], which are typically not included in the fitting of EAM potentials; and (ii) the inaccurate description of dislocation junctions. More specifically, the atomic-scale energetics and mobility of dislocation junctions (glissile, Cottrell-Lomer etc.), which play a crucial role in hardening, are rarely assessed [3]. In the last two decades, machine learning (ML) interatomic potentials have emerged [4] that are capable of reaching quantum accuracy at a computational cost that starts approaching that of empirical potentials. We can expect that, in the near future, the combination of state-of-the-art ML potentials and more efficient computing resources with the approach demonstrated by Zepeda-Ruiz et al. [1] will enable *quantitative* predictions of the hardening response based on atomic-scale mechanisms.

Discrete dislocation plasticity

In DDP the focus is on dislocation lines as the carriers of plasticity. The plastic strain rate induced by expanding dislocation loops in a given volume is determined by the rate of change of the area swept by the loops. This areal rate of change is governed by the mobility of dislocation lines and can be suppressed in various ways, thus giving rise to different mechanisms of hardening, which may be evaded by dislocation climb or cross slip. For a homogenous crystal, as investigated in the reviewed paper, the dominant mechanism is forest hardening mediated by the formation of junctions among dislocations on different slip systems. During continued plastic straining, these junctions can break when the force on the junction exceeds its strength. The nature and the associated strength of a junction depends on the relative orientation of the interacting dislocation lines and their Burgers vectors.

Within an upscaling view on multiscale plasticity, atomistic studies of unit events involved in the mentioned mechanisms have been performed in the past. Phillips and co-workers [5,6] investigated the atomic-level structure and strength of a Lomer-Cottrell junction in an aluminium single crystal. These and related studies convincingly showed that the strength of such junctions is controlled by elastic contributions outside the core region, thus making DDP a suitable approach to capture junctions, provided that the discretization is sufficiently fine to resolve the local curvature of dislocation segments at the entrance of the junction [7]. Thus, MD studies of unit events have shown to be a powerful tool for the formulation of local DDP rules for junctions [8]. Moreover, ultra-large-scale atomistic simulations like those in [1], in which many mechanisms occur simultaneously, can serve as a powerful tool for verification of DDP predictions of crystal plasticity.

Crystal plasticity

Crystal plasticity is a continuum theory based on the emerging variable of plastic slip, i.e. the average shear caused by dislocation motion within a volume element. As information regarding individual dislocations is coarse-grained out, the theory needs to be completed by a constitutive law for the plastic slip rate. Asaro and Needleman [9] proposed a power-law expression for the plastic slip rate in terms of the ratio of the resolved shear stress on the slip system and its slip resistance τ_y. To account for hardening, evolution laws for τ_y have been proposed of varying degrees of sophistication: the one in [9] was simply inspired by phenomenological macroscopic hardening, while recently more physically-based laws have been proposed (see, e.g., [10]) that account for coplanar hardening and latent hardening due to non-coplanar slip. Furthermore, because of the geometrically non-linear setting, crystal plasticity incorporates crystal rotations, including the interplay with hardening. At this stage, however, a direct connection with lower scale information is missing: the parameters of the phenomenological laws are fitted to reproduce experiments.

Compared with the state-of-the-art work on crystal plasticity, the novelty of the approach proposed by Zepeda-Ruiz et al. [1] is twofold: first, hardening is obtained by atomic-scale simulations without any as-

sumptions regarding flow rules and dislocation interactions. The macroscopic mechanical response is therefore stemming from the interatomic potential: if the potential is accurate compared with experiments/DFT, then the simulations have a predictive nature. Second, the simulations reported in [1] enable the identification of the nanoscale origin of the emergent hardening behaviour, which in crystal plasticity is effectively taken as the point of departure for the modelling rather than the result of smaller-scale physics. This enhanced understanding can be helpful in refining the formulation of hardening laws, while the computational results themselves can serve for the identification of parameter values. Also, it is conceivable that machine learning can extract hardening laws directly from these kind of atomistic studies.

Conclusion

In our opinion, the real value of this work goes much beyond the influence of crystal rotation on staged hardening. A truly remarkable impact on the field is envisioned when the richness of computational data could be unlocked to other researchers in multiscale plasticity. The most obvious value for model development, in our opinion, lies in using the data for the validation of physically-based constitutive laws used for DDP or CP. The advantage of this computational data over experimental data is the ability to query the data at multiple levels. The enormous quantity of data generated by this type of simulation (atomic coordinates of 300M atoms simulated for ~40 ns with femtosecond resolution, accessible via the Supplementary Information of [1]) is a considerable bottleneck for storage, but the information that can be retained for higher scales, such as full scale DDP simulations, can be extracted, for instance, by means of the dislocation extraction algorithm (DXA) [11]. Time sampling can be also reduced after assessing the characteristic times for dislocation events (e.g. hopping from local/Peierls barriers, unpinning from obstacles), which are orders of magnitude larger than the atomic vibrations that occur at the atomic scale.

Finally, we would like to point out that while Ref. [1] has focused on strain hardening originating from dislocation-dislocation interactions, there are numerous other sources for hardening in real metals, such as precipitate hardening. The details of dislocation–precipitate interaction can be unravelled by atomistic studies, while DDP validated on atomistics is ideally suited to capture the statistics of dislocations interacting with a distribution of precipitates.

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