MECHANISM OF DISLOCATION JAM AND STARVATION ON CRYSTAL PLASTICITY IN SUBMICRON PILLARS

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Summary Size effect at submicron scales is a crucially important issue on plasticity of materials. There are two main mechanisms that govern the plastic behavior at the submicron scales as the dimensions variation of the compressed pillars. The first is dislocation starvation induced by the annihilation of dislocations from the free surfaces. The second is forest dislocation hardening induced by the multiplication of a large amount of dislocations. The difference between the two mechanisms comes from the differences in dislocation structures. In large scale single-crystals, the jammed structure can promote dislocation multiplication (forest hardening). In small scale single-crystals, the space limitation could hinder the formation of dislocation jamming. This would lead to the breakup of dislocation structure and the dislocation annihilation process would predominate. In this paper, the critical condition of the formation of dislocation jamming is studied and the intrinsic effect for crystal plastic at submicron scale is revealed.

DISLOCATION JAM AND STARVATION

Dislocation jamming is a quasi-static state induced by the interaction of a large quantity of dislocations inside the crystal[1]. It can significantly affect the plastic behavior of crystal. The latest results indicate that the jammed structures are metastable and can be destructed by the long range mutual interactions between dislocations in a collective, avalanche-like process[2], leading to random strain bursts in micro-[3-4] and nano-crystals[5-6]. Jamming structures are usually applied to the diffusion and aggregation of point particle systems and each particle in the system is considered to be a single element, such as traffic flow, a crowd of people and granular materials, etc. In two-dimension discrete dislocation dynamic (2D-DDD) simulations, the researchers often similarly use this hypothesis, and whether a jammed state occurs is determined by the velocities or correlation length of the dislocations [1]. However, this hypothesis is invalid for 3D cases because of the interaction and multiplication of dislocations inside the crystal. Thus, in the real 3D case of the present work here, we focus on the new definition of dislocation jamming.

SIMULATION SETUP AND RESULTS

In order to examine the new definition of dislocation jamming, the compressions of two Au single-crystal micro-pillars are simulated by 3D-DDD simulations. In our simulations, the discrete dislocation plasticity is solved under a completed continuum mechanics framework, which can easily deal with the large deformation and dislocation-interface interactions [7-8]. The micro-pillars, with diameters of 250nm and 500nm, are cut from the same bulk sample and have an identical initial dislocation density ($3\times10^{14}m^{-2}$). Before compression the pillars are stress-relaxed to reach an energy equilibrium state. During relaxing, the dislocations intersect with each other and interact with free surfaces, leading to initial dislocation junction formation and annihilation. Several factors are taken into account, such as free surface effect, dislocation junction formation and dislocation topological evolution [7-8]. Besides, the stability of dislocation junctions is also considered by minimizing the system energy using a conjugate-gradient algorithm. The single-crystal material is taken to be isotropic elastic gold, with the shear modulus μ=27.5GPa, Poisson's ratio v=0.42 and static viscous drag coefficient $B_0=5.0\times10^{-5}$Pa/s. The top surface of the pillar uniformly undergoes a constant uniaxial velocity (0.1nm/s).

The two size pillars display obviously different behaviors during compression. In the 250nm pillar, almost all the mobile dislocations annihilate at free surfaces without multiplication inside the crystal, resulting in a mechanical annealed state. This state requires a higher stress to activate more sources for plastic flow. Once there are enough mobile dislocations, a stress drop would take place. On the other hand, in the 500nm pillar, it can be deformed at a relative low stress level due to the increasing storage of the mobile dislocations. With the increase of the displacement, dislocation multiplication is observed and the dislocation density has more than doubled compared to the initial state. As a result, the forest hardening occurred. The movies documenting the entire compression process are shown in supporting materials.

In dislocation-jammed system, the junctions are the crucial elements. They work as the sources of pinning points for dislocation multiplications. After initial relaxation, the junctions in both pillars are separately distributed in the crystal consisted of small amount of dislocation segments. Obviously, this structure cannot be called a junction chain. In the 250nm pillar, the density of the dislocation junctions is kept at low level when the stress is low and sharply decreases to zero once the stress is large enough. We name this junction structure as a fragile dislocation jamming. All of these junctions have a short life time. In the 500nm pillar, the initial configuration is identical to that of the 250nm pillar, i.e., the junctions are isolated structures. As the loading continues, one specific junction could break up. However, the density of dislocation junctions oscillates with an increasing trendy. At the same time, the junctions inside begin to evolve to become chain structures, occasionally some of them could form a junction loop. From a statistical point of

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view, the distribution of junctions does not change as a whole although the individual junction is not stable. Almost all of the junctions are immerged in the chain-structure, even they have different characteristics. We believe the dislocation junction-chains are crucial elements for robust dislocation jamming, and a large volume is one of the necessities for the formation of junction chains. Accompanying with the breakup of dislocation junctions, the dislocation avalanches occurs. In large samples, the junctions can self-organize to form internal chain-like structures during deformation by all kinds of dislocation interactions. During this process, as the dislocation interaction and multiplication keeping on operating, more and more junctions with different characteristics form. Thus, the dislocation interaction is another necessity for dislocation jamming.

As aforementioned, the dimension of the crystal affects the jamming of dislocation structures. Besides, the stress level and the dislocation density can also influence the formation of jamming. Liu et al. [9] established a speculative phase diagram for jamming in fragile matter. According to this 3D-diagram, taking account of the three factors for jamming structure, a possible phase diagram for dislocation jamming at normal temperature is sketched with dimension^{-1}, dislocation density^{-1} and stress level as three coordinates, as shown in Figure. The super-surface represents the critical condition of forming dislocation jamming: transition size, nucleation stress and nucleation dislocation density for jamming. The interior of the surface represents the region that jamming can form, while the exterior represents the region that cannot. From the diagram, the stress decrease, dimension increase and density increase could all be beneficial to the formation of dislocation jamming.

To verify the correctness of the trend of the diagram, four verifying examples (the compression of Au micro-pillars) are given. First, the initial dislocation density is set to be $3.0\times10^{14}m^{-2}$ and the stress levels in both compressed 250nm and 500nm pillars are fixed to be 0.5GPa. The simulation results show that dislocation jammed state has been formed in 500nm sample (Example 1), while mechanical annihilation has occurred in 250nm sample (Example 2). Then, the dimension is fixed at 500nm and the stress is increased to 5.0GPa (Example 3). In this case, all the dislocation junctions are broken up and the mobile dislocations escape from the free surfaces. At last, the diameter of the micro-pillar is set to be 500nm and the relationship between the initial dislocation density and the jamming state formation is studied. If the stress is kept as 0.5GPa and the initial dislocation density is decreased to $0.8\times10^{14}m^{-2}$, dislocation jamming would not occur due to the lack of enough stable dislocations.

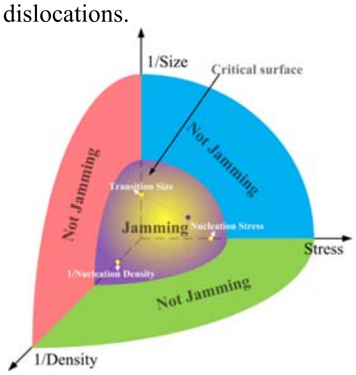

Figure Super-surface sketch for the critical condition of forming dislocation jamming

CONCLUSION

The dislocation junction chain structure is the necessity of forming dislocation jamming, while robust dislocation jamming is crucial to forest hardening and generates a smooth stress-strain curve. If the crystal is absent of jamming, the plastic behavior would be in an intermittent state.

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