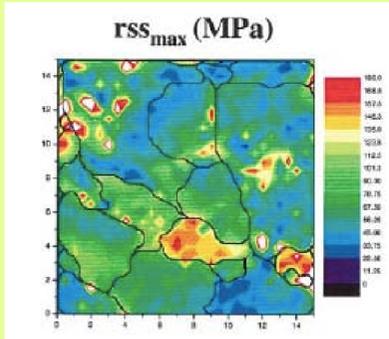


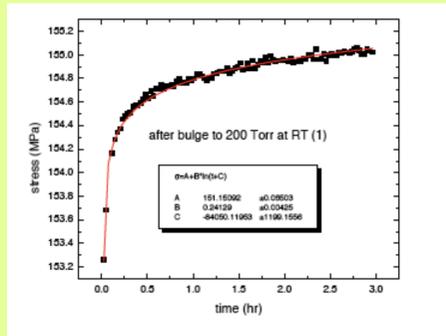
Plastic strain recovery in nanocrystalline thin films.

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Understanding the mechanical response of thin films is essential to improve the reliability of microdevices. In MEMS devices thin films are subjected to stresses due to the fabrication process, the difference in the thermal expansion coefficient of the components and the stress due to the film deformation during operation. Predictive models should include the effect of the microstructure in the local stress that influence the long term operation of MEM devices.



Critical resolved shear stress in a Cu thin film (2).



Reverse stress relaxation in a Cu thin film (4).

The effect of the grain size distribution in the mechanical response has not been well established. Recent experiments in nanocrystalline thin films show that plastic strain is recovered under macroscopically stress-free conditions. The authors suggest that a broad grain size distribution produces a highly heterogeneous stress distribution and this is responsible for plastic strain recovery.

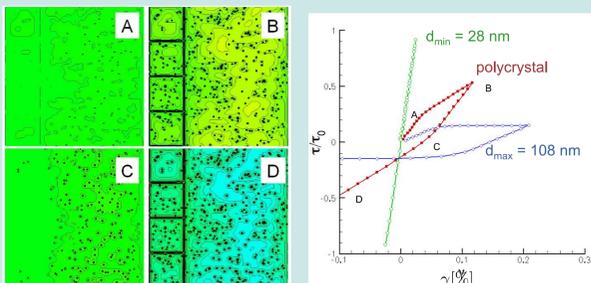
Rajagopalan *et al.* (1) conducted experiments in nanocrystalline aluminum and gold thin films with an average grain size of 65 nm and 50 nm, respectively. Both materials recover 50–100 % of plastic strain after unloading. Another feature observed in these experiments is that once the strain is recovered the specimen shows no residual hardening during the next loading. X-ray and deformation studies on crystalline aluminum with a bimodal distribution of grains with grains in the range 40–400 nm also suggest that plastic strain recovery requires the presence of sufficiently small and big grains to generate inhomogeneous stress distribution in the sample (3). These findings reveal that the average grain size itself is not enough for a complete characterization of the microstructure in nanocrystalline materials but the grain size distribution should also be considered.

Grain size distribution effects in nano-crystalline materials

Plastic deformation is size dependent, this is observed in experiments and simulations and has a fundamental effect in crystalline materials with average grain size in the nanometer range. Recent experiments show that plastic deformation is not only affected by the average grain size but also by the grain size distribution. One of most notorious aspects is that nanocrystalline metals recover plastic strain after unloading. Here we perform numerical simulations that show that plastic strain recovery in nanocrystalline materials is driven by the inhomogeneous stress distribution observed in samples with large grain size distribution.

Phase Field dislocation simulations

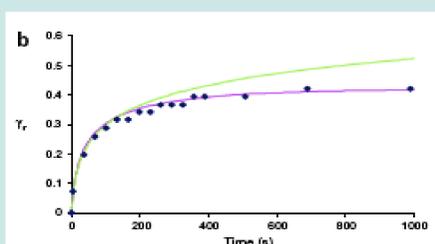
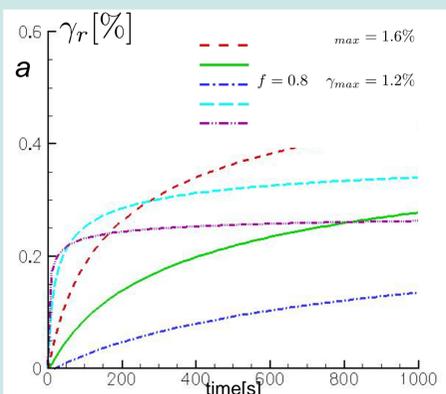
We present dislocation dynamics simulations of plastic deformation of polycrystalline materials with a bimodal distribution of grains. The simulations show that small grains deform elastically while bigger grains deform plastically causing a inhomogeneous distribution of strain in the sample. After removal of the applied stress the small grains remain in tension while the big grains are in compression. Therefore, at macroscopically zero stress dislocations are under the influence of local stresses and by a thermally activated depinning relax the energy of the system resulting in macroscopic strain recovery. This effect is observed in our simulations only in the presence of heterogeneity in the size distribution in agreement with experiments (1,2).



Simulated dislocation patterns and stress-strain curve for the macroscopic polycrystal (filled squares) and local stress strain curves for the individual grains (open symbols) (5).

Creep deformation

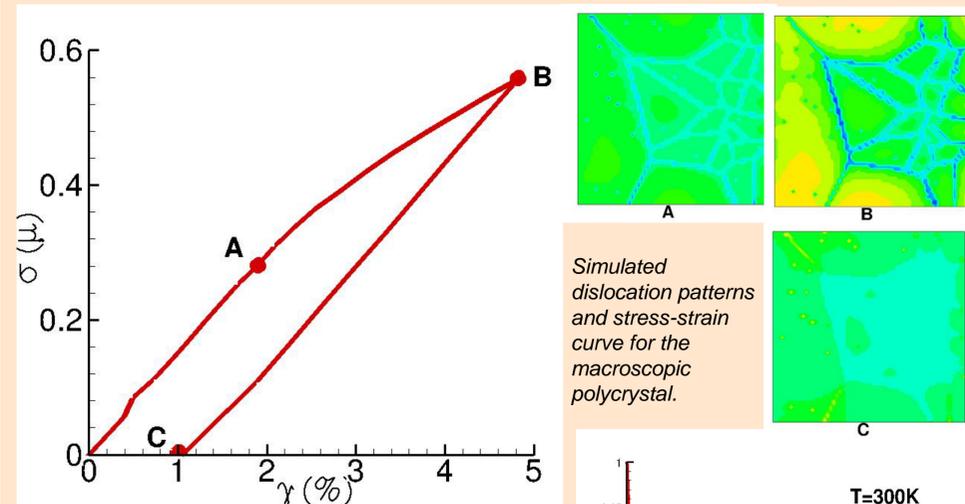
After removal of the macroscopic stress the system evolves by relaxing the heterogeneous stress distribution by creep deformation.



(a) Simulated plastic strain recovery (5) and (b) Experimental plastic strain recovery (1).

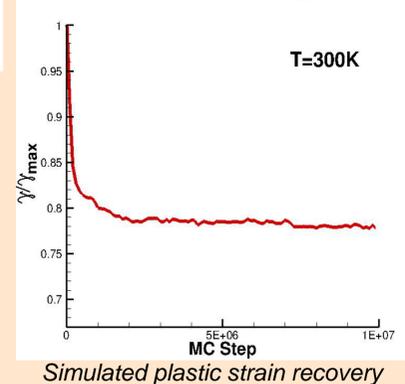
Metropolis Monte Carlo simulations of creep recovery

In this section the phase field dislocation dynamics code is coupled to a Metropolis Monte Carlo algorithm to study plastic strain recovery. Proceeding to the numerical solution of the phase-field dislocation model, the slip plane is discretized in a square of 200 by 200 grid points with periodic boundary conditions and a random array of obstacles. The grain boundaries are impenetrable to dislocations.



The simulations are performed with a Metropolis Monte Carlo algorithm using a transition probability that accounts for the energy of the dislocation ensemble.

The polycrystal is loaded up to B and then the stress is released (point C). The system relaxes the strain in the large grain by creep deformation.



Summary and future work

That plastic strain recovery is caused by a grain size distribution has important implications for the interpretation of deformation mechanisms in nanocrystalline materials with applications in MEMS. It was suggested that plastic strain recovery is driven by grain boundary accommodation. Our simulations do not include this mechanism but yet predicts the correct behavior. This implies that plastic strain recovery may be driven by a combination of both mechanisms but at room temperature and with grains in the 10nm-100nm range the plastic deformation of big grains surrounded by elastically deforming small grains are the dominant mechanisms as suggested also by atomistic simulations.

Most important, the present results reveal that average grain size itself is not enough for a complete characterization of the microstructure in nanocrystalline materials but variations in the grain size distribution should also be considered. Future work includes characterization of the effect of the uncertainty in the grain distribution in the amount and rate of plastic strain recovery.

References

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