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Theoretical modelling of grain boundary anelastic relaxations

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Abstract

Grain boundary stress relaxation in Au polycrystals and single crystals has been studied by mechanical spectroscopy. A relaxation peak related to grain boundaries is observed at 620 K. Molecular dynamics simulations on Au are performed in order to illustrate the potential microscopic mechanisms responsible for the stress relaxation peak in Au polycrystals. A Σ5 grain boundary is submitted to a shear deformation parallel to the boundary plane. In agreement with previous studies on Cu, the grain boundary shows a migration perpendicular to the boundary plane coupled to shear for temperatures below 700 K. Above 1000 K, only grain boundary sliding occurs. Two models are developed that provide expressions for the relaxation strength Δ and the relaxation time τ that are compared to experimental measurements performed on polycrystals. The observed grain size dependence of Δ and τ favours the sliding model over the migration model.

Keywords: Grain boundary sliding; Coupled migration; Gold; Molecular dynamics; Internal friction

1. Introduction

Grain boundaries (GBs) play an important role in the mechanical properties of metals. Especially in fine-grained materials, where the GB density is high, GBs determine the plasticity. A key mechanism for deformation at high temperatures is grain boundary sliding (GBS). This mechanism has been shown experimentally in ultrafine-grained Cu [1], Al [2], Au thin films [3] and AuPd nanocrystalline materials [4]. The deformation mechanism was observed indirectly, since the experimental techniques are mostly tensile tests and indentation tests. Direct observation of GBS has been made on single incommensurate boundaries in nanopillars [5].

Another deformation mechanism acting on the GBs that was observed in various metals is the so-called coupled GB motion, where a shear deformation parallel to the boundary plane is accompanied by a normal boundary migration. In symmetrical low-angle tilt GBs, this deformation mechanism can be easily understood as a collective glide of edge dislocations [6]. The shear stress acting parallel on the boundary causes a glide force on each GB dislocation which results in a migration of the boundary plane. In GBs with higher miosorientations, the dislocation model is no longer applicable, but theoretical analyses by Cahn et al. [7,8] and Caillard et al. [9] predicted a coupled GB motion to also occur in the case of high-angle GBs. Coupled GB motion has been observed and studied experimentally in bicrystals in pure Al [10–12] and in Zn [13]. The activation energies depend strongly on the GB type, e.g. the misorientation angle.

Mechanical spectroscopy is an experimental technique that measures the energy loss during a cyclic deformation caused by the movement of crystal defects such as dislocations or grain boundaries. It therefore monitors the dynamics of a stress relaxation process. It is well known that the presence of grain boundaries influences the high temperature mechanical loss spectrum in metals showing

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a mechanical loss peak at approximately half the melting temperature [14–19]. The microscopic mechanism causing this relaxation peak is not well understood. Woirgard et al. [20,21] concluded that damping mainly originated from lattice dislocations, whereas a study on Al bicrystals [22,23] showed that the relaxation peak was only present in samples containing at least one GB. Moreover, the peak depended on the misorientation of neighboring grains.

In 1941 the first model predicting a relaxation peak due to GBS was developed by Zener [24]. The model predicted that the peak height should not depend on the grain size d. The only parameter influencing the peak amplitude was the Poisson's ratio. It turned out that the peak height predicted was too large by a factor of 5 for most materials. The Zener model considered a polycrystal composed of spherical grains, which do not fill the space. The kinetics of the Zener model were discussed in REf. [25] under the assumption that the shear stress is reduced to zero at the boundary and that the anelastic strain compensates the elastic strain.

Raj and Ashby [26] modelled the creep rate of a polycrystal considering GB regions as a wavy surface with a slip viscosity η. Morris [27] and Lee [28] calculated the mechanical loss spectrum of a polycrystal, adding the contribution of grain boundaries according to the Raj–Ashby model. The model set-up was rather complicated and did not provide a simple formula for the mechanical loss containing, for example, the grain size d or the GB viscosity η, which would permit a direct comparison to experimental findings.

A recent study of the GB peak in yellow gold alloy [29] measured a grain size exponent $m = 1$, which means that the relaxation time τ of the underlying microscopic mechanism scales linearly with the grain size. Moreover, the peak amplitude did not change with grain size. This was a confirmation of the Zener model, which is a purely geometrical model. However, the nature of the microscopic mechanism causing the GB relaxation peak is not discussed.

Molecular dynamics (MD) computer simulations on the subject of coupled GB motion have been performed by Mishin et al. [8,30], Elsener et al. [31] and Homer et al. [32]. The simulation study on Cu bicrystals in REf. [8] showed that, for various high-angle tilt GBs, the deformation behaviour changed from coupled GB motion to GBS upon heating. Furthermore, the transition temperature depended on the tilt angle.

There are two other possible phenomena associated with GBs: grain rotation and GB migration without associated shear deformation. These two mechanisms are not driven by an external shear stress and would not cause a stress relaxation in the case of homogeneous shear stress.

The experiments of coupled GB motion are mainly performed on isolated boundaries and are compared with MD simulations. These simulations give access to the position of every atom during the simulation and are well adapted to the study of microscopic mechanisms related to GBs. On the other hand, simulations are limited by the sample size to a single GB or a few nanoscale grains [33,34]. It is difficult to judge from a MD simulation whether the observed mechanism, such as GBS or coupled motion, is also active in a real polycrystalline material and to what extent it contributes to the mechanical properties of the material.

Since gold alloys have been shown to produce GB peaks [35,36], pure gold is investigated in the present study. Effectively, the mechanical loss spectrum of 4N Au polycrystals shows a GB peak. MD simulations are used to illustrate the possible microscopic relaxation mechanisms that act at a GB. One specific boundary type ($\Sigma5$) is chosen in order to show the existence of shear coupling at low temperatures and GBS at high temperatures under a shear deformation in pure gold.

It is important to simulate the same material as used in the experiment because mechanical spectroscopy is a very sensitive technique for probing the microstructure and the elemental composition. Small variations in the composition of the material can change the mechanical loss spectrum drastically [37,35]. The $\Sigma5(310)$ tilt boundary has been chosen as a model boundary because its boundary energy shows a local minimum in the energy landscape [38]. The probability of finding the same boundary type in the polycrystalline sample is therefore higher than that of finding a random GB.

In the second part of this paper, two models are developed to describe the mechanical loss spectrum of the polycrystal. The first model is inspired by a coupling mechanism that causes the GB to migrate under an applied shear stress. The second model supposes that GBS is the relaxation mechanism. The explicit expression of the mechanical loss peak contain parameters that can be directly derived from the experimental results, such as the grain size d, the viscosity η and the misorientation angle θ of adjacent grains.

2. Experiments

In a deformation experiment, an external stress is applied on a specimen and the deformation is measured. For deformations below the elastic limit, where no plasticity occurs, the total strain is the sum of two contributions:

$$\epsilon_{tot} = \epsilon_{el} + \epsilon_{an} \tag{1}$$

where the elastic strain ϵ_{el} is recovered instantaneously upon unloading. The anelastic or viscoelastic part ϵ_{an} contains a time dependence described by a relaxation time τ. In the limit $t \to \infty$, the anelastic strain is fully recovered.

Mechanical loss is caused by anelastic relaxation in a material. The lag of the strain response with respect to an applied cyclic stress is a direct measurement of the energy loss. In the present study, the experiments were performed in a torsion pendulum, where a periodic stress with frequency f is applied on the sample. The phase lag $\tan(\phi)$ (mechanical loss) between stress and strain is measured directly. The ratio between stress and strain provides a measurement of the dynamic shear modulus G. If the relaxation process is characterized by a certain relaxation time τ,