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Theoretical Considerations about Grain Boundary Migration in FCC Metals

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Abstract The grain boundary motion (gbm) is not yet well understood even in pure fcc metals like Au, Cu and Al. Compared to dislocation motion, which can be distinguished in jerky and viscous motion, the movement of grain boundaries can be classified in similar ways. A video movie of an in-situ- experiment, which was obtained by high-resolution transmission-electronmicroscopy (HRTEM), shows vibritations of a 29.7°-(100) symmetrical tilt grain boundary in a thin Gold foil [1]. The interpretation of this experiment suggests to describe the grain boundary motion with a frequency and an amplitude. Equivalent sets of parameters are e.g. an effective mass and a spring constant. The static and dynamic energies are compared to literature values. These considerations lead to a coarse classification of grain boundaries into four classes according to their magnitude of static and dynamic energies, which has consequences for especially the mobility.

Introduction The understanding of the phenomenon of grain boundary migration on atomic scale is still an unsolved problem. Five different mechanisms have been found: 1) A lot of early theories about grain bondary migration consider jumps of single atoms, which are assumed to be uncorrelated [3]. 2) Jerky movement, where the grain boundary sometimes stops and waits before the motion starts again, is the most often observed mechanism of gbm [4, 5]. 3) The collective change of the atom orientation from one grain to the other similar to the martensitic transformation is an activationless motion [6]. In computer simulations this phenomenon of sudden, collective bowing out of atoms into the neighbor grain was also observed [7]. 4) In molecular dynamics computer simulations also the boundary planes often vibrates due to the thermal energy [8]. This result suggests, that the boundary plane is not really fixed, which is consistent with the observation of low activation energy for migration. 5) Migration by climb- and glide- movement of secondary grain boundary dislocation (SGBD) [5, 9, 10] or facets [11,12] is frequently observed especially in Copper, which will move perpendicular to the boundary plane.

The most important parameter for charaterization grain boundaries is their energy, which is the energy difference between the crystal with and without grain boundary [14, 15]. This is a static

energy and depends mainly on the structure only weakly on the temperature. On the other hand, in the experimental measurements on the dynamic properties of migrating boundaries an activation energy for migration can be elucidated from the arrhenius plot of the temperature dependence [2], which is therefore a dynamic energy. In some experiments the activation volume of the grain boundary migration can be measured as well, which is related to the number of atoms which are involved during a movement of the grain boundary. The goal of this paper is to compare experiments of gbm with theoretical considerations and get a better description of the atomic movement of grain boundaries.

Experimental Results Bicrystals of Gold were produced as described in detail elsewhere [1] by the well known diffusion bonding technique developed by Schober and Balluffi [16]. The Au-bicyrstal with an orientation of 29.7° was carefully heated such that the twist boundary changed into tilt boundaries which were fixed by pores. Using HRTEM on a JEOL 4000EX under Scherzer conditions of "atom contrast" [17] the gbm was recorded on video tapes with the standard rate of 4

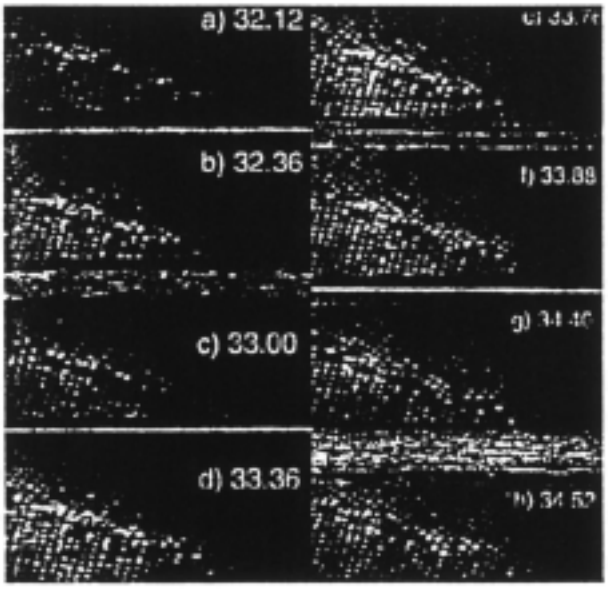

Fig 1) HRTEM-video-frames after time steps as indicated.

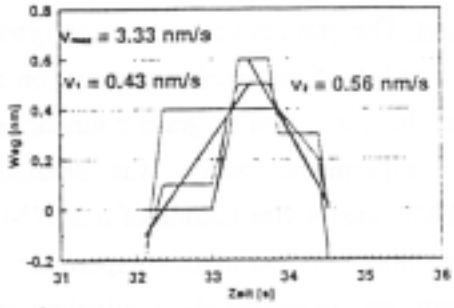

Fig. 2) Position versus time diagram for gbm of fig 1. for measuring the velocity of the gbm vibrations

frames per second and quantitatively analysed frame by frame [1].

Fig. 1 shows the HRTEM-video frames after time steps in seconds as indicated, which were obtained from the 29.7° (100) Au tilt grain boundary observed at room temperature. The video clearly shows forward and backward motions of atomic columns around an equilibirum position. It cannot be excluded that electron beam radiation supports the gbm. The vibrations were analysed in detail and the position versus time diagram (fig. 2) was plotted. Two velocities can be obtained: the maximal velocity from one position to the next $v_{max} = s_1 / t_1$, where s_1 and t_1 mean the shortest distance respectively time between a single jump. The second velocity is that for continuous migration, that means an average over several jumps $\bar{v}$. Quantitative measurements on the video tapes were perfomed for several cases and are equivalent to the results shown in the example of fig. 1. In all cases the average velocity is usually related to the maximal velocity by $\bar{v} = 1/10 \cdot v_{max}$.

Discussion After computer simulations have predicted vibrations of grain boundaries, the results of this work clearly gave the experimental evidence. These vibrations which can be compared to the

motion of dislocations and lead to the following considersations. The static and dynamic energies of grain boundaries can be explained if the atoms in the core of a grain boundary are considered. The number of atoms N which are jumping across the grain boundary plane during a certain time step is an important parameter for gbm. This parameter can also be expressed as the activation volume of gbm V or as mass of atoms m and can be calculated from the mass of each atom m_i by: $m = N \cdot m_i$. The atoms in the gb core possess bonds to the single crystal (bulk) regions on each side of the grain boundary. Hence, the vibration of the atoms in the grain boundary core can be treated in analogy to vibrations of a mechanical pendulum: The potential and kinetic energy for this case is $E_{pot} = \frac{1}{2} \cdot k \cdot x^2$, $E_{kin} = \frac{1}{2} \cdot m \cdot v^2$, (1), where k is the spring constant, x the deviation of the equilibrium position, m the mass of the core atoms and v the velocity. The solution for this problem leads to the equation of motion $x = a \cdot \sin(\omega \cdot t)$, where the eigen frequency ω depends on the mass and the spring constant $\omega = \sqrt{k/m}$ (2).

The conclusions of these considerations are straightforward, if the static and dynamic energies of symmetric tilt boundaries in Al are compared (fig. 1). Four types of grain boundaries can be distinguished according to their magnitude of energies: 1) a large dynamic energy and small static energy are possess by all small angle grain boundaries (SAGB). In the picture of the pendulum this corresponds to a large mass and a small spring constant. After equation (2) this corresponds to a small vibrational frequency ω. This is probably the reason why SAGB are stable and are known to be difficult to move during recrystallization. 2) a small dynamic energy and large static energy possess grain boundaries around Σ13-22°[001], Σ17-27°[001], and 26°[110] . The corresponding parameters are a high spring constant which means a high stiffness and a small mass, and hence only a little number of atoms are involved in the migration. The frequency of vibrations after eq. (4) is small. The symmetrical 29.7°[001] tilt grain boundary which was observed by in the reported in-situ-HRTEM-experiments as described in the previous chapter obviously belongs to this class. The observed frequencies of about 3 seconds for one vibration is indeed rather small compared to the Debye frequency of atoms. Hence, this result support the theoretical considerations. A small dynamical energy would also explain that obviously the kinetic energy at room temperature (usually 1/40 eV) is enough to let the grain boundary vibrate. 3) a (relatively) small dynamic energy and (relatively) small static energy in the sceme of fig. 4 belongs to Σ 3 and Σ 5 grain boundaries.

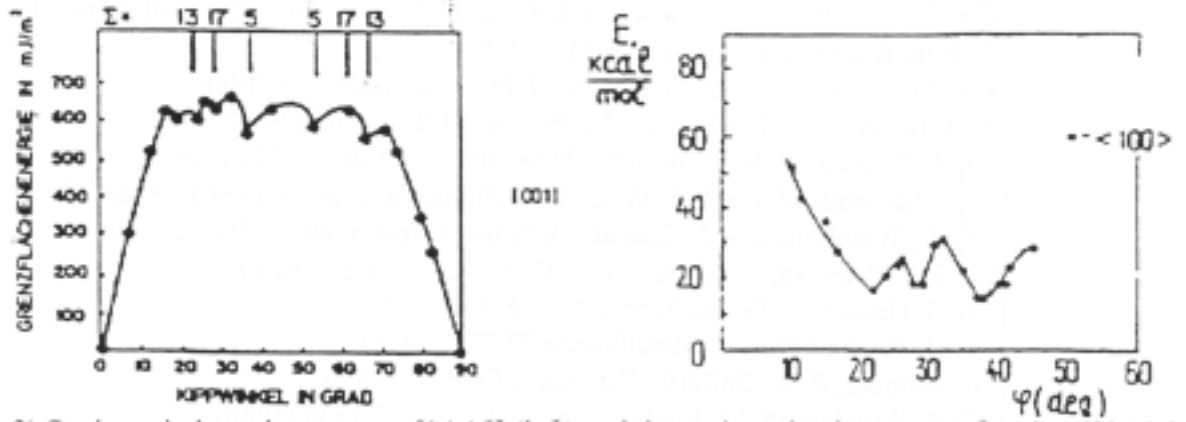

Fig. 3) Static grain boundary energy [14,15] (left) and dynamic activation energy for gbm [2] (right) of symmetrical tilt boundaries in Al for (001) orientation as a function of the tilt angle.

Finally, the fourth case 4) large dynamic and static energies will correspond to the so called random grain boundaries. For the cases 3) and 4) the frequencies have middle values, because either the mass or the stiffness are high or low.

Modelling the five different mechanisms of gbm's on an atomic scale requires an classification by at least three independent parameters [1], as there are: „number of atoms N involved in a jump", „jumping distance of the boundary plane during a certain time step", and finally „time sequence of subsequent jumping events". The later parameter is controlled by the waiting time at an obstacle and is related to the ratio $v_{max} / \bar{v}$. Neglecting the fifth mechanism, the migration of a facetted step by climb and the glide of the SGBD, which is probably a special case, four usual mechanisms of grain boundary movements can be distinguished. The energetic considerations lead also to four cases. Therefore, it makes sense to compare the four mechanisms with the four classes of dynamic and static grain boundary energy. The „diffusion controlled jump of single atoms" has a low mass, while the „martensitic-like collective movement of atom groups" has probably the highest mass. The comparsion of the movement of grain boundaries with a pendulum is of course valid for the reversible movement as explained with the observed vibrations at room temperature. The recrystallization will happen with a small irreversible bias force, which means that the atoms in the gb core will break the atomic bonds to the bulk atoms.

Conclusions 1) For the first time vibrations of a 29.7° (100) tilt grain boundary in Au has been experimentally observed by in-situ-HRTEM-video-tapes. These vibrations have been also been found in molecular dynamics computer simulations. 2) Vibrations of grain boundaries can be compared to vibrations of a mechanical pendulum, if an effective mass and a spring constant is introduced. 3) Grain boundaries can be charaterized into four groups by comparing the static grain boundary energy with the dynamic activation energy for migration.

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References

[1] W.Wunderlich, G. Gottstein, to be published
[2] G. Gottstein, L.S. Shvindlerman, Scripta Metall. Mat. **27** 1515-1520, 1521-1526 (1992)
[3] F. Haessner, Journal de Physique, **C4** C4-345-354 (1975)
[4] S.E. Babcock, R.W. Balluffi, Acta metall. **37** 2357-2365, 2367-2376 (1989)
[5] R. Scholz, C.L. Bauer, Coll. de Physique **C1** C1-623-628 (1990)
[6] C.V. Kopetskii, V.G. Sursaeva, L.S. Shvindlerman, Sov. Phys. Sol. State **21** 238-240 (1979)
[7] Jhan, Bristowe Scripta Met. 1313 (1990),
[8] C.Counterman, Chen, G. Kalonji, J. Phys. Coll. C5-139 (1988)
[9] H. Ichinose, Y. Ishida, Coll. de Physique **C1** C1-185-190 (1990)
[10] R. Würschum, R.W. Balluffi, Phys. stat. sol. **126** 323-336 (1993)
[11] T.Muschik, W.Laub, U.Wolf, M.W.Finnis, W.Gust, Acta met. mater. **41** 2163-2171 (1993)
[12] W. Wunderlich, H.J. Gudladt, Acta metall mater. **40** 2123-2129 (1992)
[13] B.C. Petersen, U.Czubayko, G. Gottstein, to be published
[14] G. Hasson, C. Goux, Scripta Met. **5** 889 (1971)
[15] H. Fischmeister, Z. Metallkunde **77** 771 (1986)
[16] Schober, R.W. Balluffi, Thin Solid Films 1 (1976)
[17] W.Wunderlich, M. Ruehle, Proc. ICEM 1335-1336 (1986)