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Quantitative Determination of Interface Structure by Transmission Electron Microscopy Techniques

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Many properties of polycrystalline materials are controlled by the structure and composition of internal interfaces. It is therefore desirable to know the characteristics of those lattice defects. Different transmission electron microscopy techniques allow the determination of all parameters of interface structure and composition. This can in most cases be performed only for very short segments of rather special boundaries fulfilling specific geometrical constraints.

Further, theoretical simulations of interface structures result in interface structures which can be compared to experimentally determined structures of equivalent grain boundaries or interfaces.
This procedure sounds simple and straightforward. It has to be kept in mind that there exist several major problems which have to be overcome.-

Bi-crystals of different materials were prepared in a UHV bonding machine [1]. Metal-ceramic interfaces were primarily formed by MBE growth of thin metallic films on single-crystalline substrates (Cu/α-Al_2O_3, Nb/α-Al_2O_3, Pd/ZnO, …). Specimens suitable for TEM studies were prepared from the bulk material and were investigated in a high-resolution TEM (without C_s-corrector).

Fig. 1 shows as an example micrographs used for the determination of the structure of a symmetrical tilt grain boundary in α-Al_2O_3, Σ11 $(\bar{2}116)$ in $[0\bar{1}\bar{1}0]$ projection. Fig. 1a represents the translation-averaged image, Fig. 1b displays the simulated micrograph of the structure (Fig.2) resulting in the best match between experimental and simulated image. Fig. 1c is the difference image of Fig. 1a and 1b,. The agreement between Fig. 1a and 1b is very good, proving that the grain boundary structure shown in Fig 2 and used for the simulation of Fig. 1b is close to the actual structure. The simulated structure is generated by shifting the two crystals juxtaposing at the interface against each other and by the relaxation of individual columns. Error bars can be evaluated [2].
Detailed analyses were performed for a group of grain boundaries and the results were compared to the results of simulations [3]. Deviations are within the error bars.

A corresponding analysis of general grain boundaries by quantitative HRTEM is not possible. Also, it is unclear if the results for special grain boundaries are of any relevance for polycrystalline alumina.
Pd and $SrTiO_3$ form a coherent phase boundary. Q-TEM can be used to determine the distance T_3 between the terminating layers [4]. Since in this case an image averaging is possible, this value can be obtained with high precision.

References:

1. H.F.Fischmeister et al, Rev. Sci. Instruments, **64** (1993) 234.
2. G. Richter and M. Rühle, Interface Science, 12 (2004) 197.
3. A.G. Marinopolous and C. Elsässer, Acta Materialia 48 (2000) 4375.
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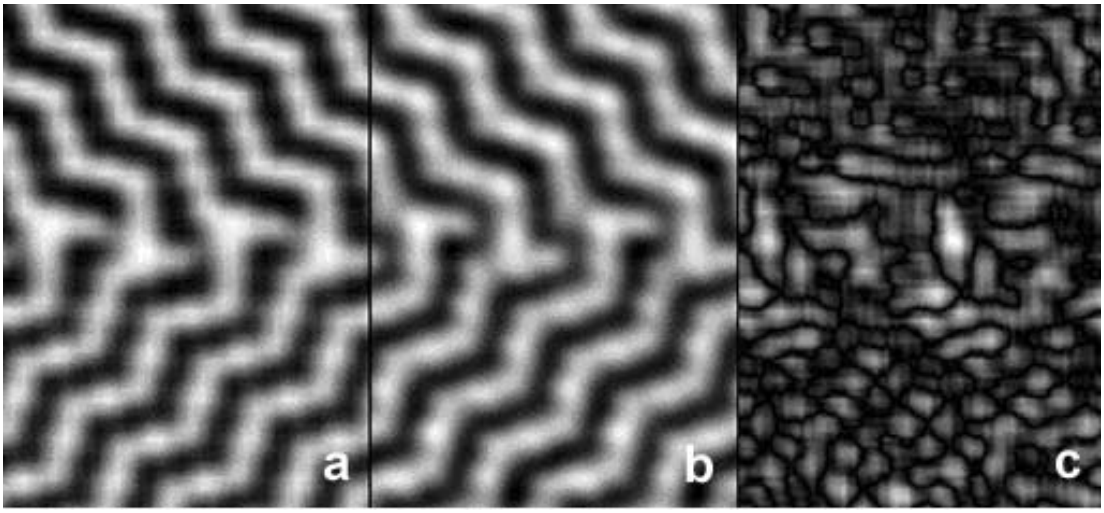

FIG. 1. Analysis of a symmetrical tilt grain boundary ($\Sigma 11\,(\bar{2}116)$ in alumina, $[01\bar{1}0]$ projection)
The $(\bar{2}116)$ interface plane is oriented horizontally in the middle of the micrograph
a) Experimental image, translation-averaged
b) Calculated image (using structure depicted)
c) Difference of Fig 1a and 1b, enhanced by a factor of 5

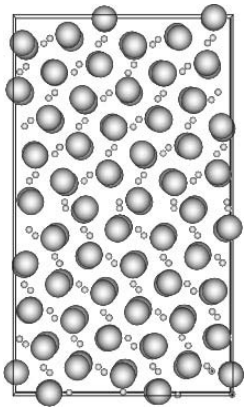

FIG. 2. Atomic structure of grain boundary of Fig 1

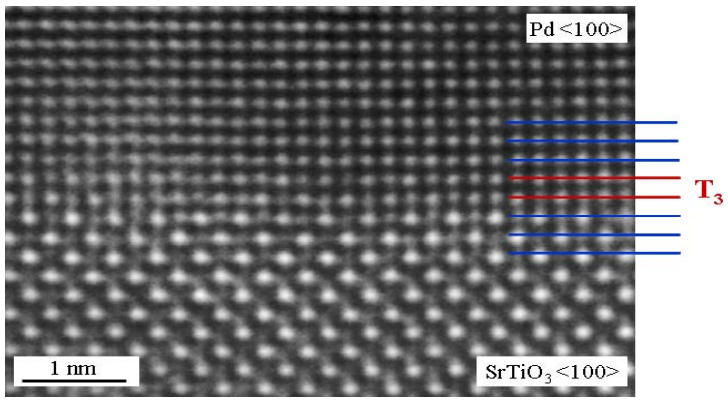

FIG. 3. Coherent Interface between Pd and $SrTiO_3$
Translation vector T_3 = (0.255 + 0.005) nm