

**PS10.08.22 X-RAY DIFFRACTION OF INTERFACES IN NANOCRYSTALS.** Yuming Wang and Kai Xing, Department of Materials Science, Jilin University, Changchun 130023, PR China

Fe and its oxides have been made in the form of nanocrystalline powders. The chemical as well as the vacuum deposition technologies were used to produce a great variety of microstructure, such as with different grain size, internal strain and inhomogeneity. The whole X-ray diffraction patterns of these samples were processed by Rietveld analysis using DBWS-9411 code supplied by Prof. R.A. Young. On the other side, the interfaces of these nanocrystals were simulated by molecular dynamics with several theoretical structural models. After sufficient atomic relaxation the interface structure reached equilibrium. Then the theoretical effect of interfaces on the whole X-ray diffraction pattern can be evaluated in detail. The comparison between the theoretical and experimental diffraction patterns gave a possibility to select the correct structural models as well as the interatomic potentials and related parameters. Using the correct interface structure one can predict a series of physical and mechanical properties of nanocrystals on a much sounder basis as compared to usual methods. This is important especially for those properties which are very difficult to measure experimentally.

**PS12.01.22 GRAIN BOUNDARY CRYSTALLOGRAPHY.** D. Romeu, L. Beltrán, J.L. Aragón, A. Gómez. Instituto de Física, UNAM, Apartado Postal 20-364, D.F. 01000 México

In this work we present a mathematical model capable of describing in detail the atomic structure of arbitrary grain boundaries (GB) in metals and other materials and constitutes the first step towards a complete crystallographic description of GBs. Due to its evident technological implications, GB have been intensely studied in the past with limited success, due, mostly, to the absence of a complete model accounting for the structure of arbitrary GB. This has hampered the establishment of a correlation between boundary structure and properties.

Using tools closely related to those used in Quasicrystals, the present model describes in detail the atomic structure of arbitrary GB, not being restricted to those known as "special" and establishes a link between the fields of quasicrystals and GB, permitting a better understanding of both. The model replaces the notion of "coincidence sites" by "best possible fit" and it is continuous (as the O-lattice) over all the angular range.

Our results show that the value of Sigma alone is not enough to characterize special boundaries. In particular, it has been found that some low Sigma GB in FCC metals have a very poor fit (Sigma 17) while others with higher Sigma are surprisingly good (Sigma 41), thus explaining previous experimental results indicating that Sigma 41 is a special boundary.

**PS12.02.31 STRUCTURE OF SiC FILMS GROWN ON Si(111) AND (110) SUBSTRATES BY SOLID-SOURCE MOLECULAR BEAM EPITAXIE.** U. Kaiser, A. Fissel, W. Richter, S. B. Newcomb\*, W. M. Stobbs\*, Institut für Festkörperphysik, Friedrich-Schiller-Universität Max-Wien-Platz 1, D-07745 Jena, \*Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge, CB2 3QZ

TEM and AFM studies have been carried out to demonstrate the influence of growth parameters and substrate orientation on the structure of SiC films deposited simultaneously and alternately from two sources by solid-source molecular beam epitaxy at low substrate temperatures (750 C-900 C). At 750 C and high growth rates (>2nm/min) polycrystalline columnar films were grown which show a weak orientation relationship to the substrate. While growing the films under conditions for Si stabilization at the surface and over the substrate temperature range of 800 C to 850 C at high rates, the films are strongly textured but still grow with a columnar morphology. Clear evidence for the outdiffusion of Si from the substrate is found, leading to porous regions in the substrate

at temperatures up to 800 C and to voids above 800 C. At growth rates below 1nm/min and a certain adatom ratio the nucleation mode changes from 3 to 2 dimensional and single crystalline epitaxial cubic films were grown. The influence of the adatom ratio Si:C on the growth and on the defect formation is discussed at 3 different Si:C adatom ratios (0.95, 1.05, 1.20). When the layer is deposited under slow and less kinetically controlled conditions using an alternating supply of Si and C controlled to the atomic plane level, single crystalline cubic SiC films with very flat surfaces are formed which tend to establish the hexagonal polytype. Differences in the growth on (111) and (110) substrates might be expected and are discussed as result of the differing crystallographies at the interface.

**PS16.02.17 INTERFACE KINETICS AND MECHANISM OF A NEW ORGANOMETALLIC COORDINATION COMPOUND: ATMB CRYSTAL.** Xiling Yu, Yi Sun, Wenbo Hou, Shujun Zhang and Zhenxiang Cheng, The State Key Lab. of Crystal Materials, Shandong University, Jinan 250100, P.R.China

The interface growth kinetics and mechanism of organometallic coordination compound-trialllylthiourea mercury bromide (ATMB) crystal have been studied, for the first time, by using real-time microscopic analysis system. The velocity V of straight line step trains movement and normal growth rate R of the crystal face have been measured in situ. The space between step trains is larger (from 2  $\mu\text{m}$  to 15  $\mu\text{m}$ ) while the height is lower ( $h=0.04-0.25 \mu\text{m}$ ). The direction of steps movement is vertical to the step trains. The results are given following from the model of multiple two-dimensional (2D) nucleation. The specific free energy of the step riser per unit surface of the riser is about 0.05 (J.cm<sup>-2</sup>). The relationship between the velocity V of steps and supersaturation  $\sigma$  is nonlinear. This is not in agreement with the classical theory of the layer-2D nuclei growth, since it is based on the linear relationship. This problem is also discussed.

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**PS21.02.09 DETERMINATION OF ZERO-FLUX SURFACES AND INTEGRATED PROPERTIES FROM EXPERIMENTALLY DETERMINED CHARGE DENSITIES IN CRYSTALS.** C. Flensburg, D. Madsen, S. Larsen and R.F. Stewart, <sup>a</sup>Centre for Crystallographic Studies, University of Copenhagen, Denmark, <sup>b</sup>Department of Chemistry, Carnegie-Mellon University, Pittsburgh, U.S.A

Topological analysis of electron densities is a well established method in theoretical chemistry used to characterize atomic properties and interatomic interactions. Recently it has been shown that the topological analysis also can be applied to theoretical electron densities in crystals. We have investigated topological features of densities determined from projection of X-rays diffraction data onto the multipole model. The number of different types of critical points (CP) in the unit cell must satisfy the Morse equation. The asymmetric unit is scanned for places where the gradient of the electron density vanishes and sets of CP's that satisfies the Morse equation are found. A topological atom is defined as the union of an attractor and its associated basin. The basin being the volume enclosed by the surface which has zero-flux in the gradient of the charge density. We have implemented an algorithm analogue to the promega method. Results from integration of properties of topological atoms in crystals for several systems will be presented.