

Electron Tomographic Characterization of ErSi_2 and $\text{Ge}_x\text{Si}_{1-x}$ Nanoparticles Prepared by Doping of 4H-SiC

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Small semiconductor or transition metal crystals embedded in a semiconducting matrix are nanostructured systems with interesting new properties in fields such as optics and spintronics. Ge nanocrystals embedded in SiC are, for instance, a promising system for optically active quantum dots. In addition to their size, composition and strain, their electronic structure strongly depends on their shape [1]. We have studied the 3D structure of $\text{Ge}_x\text{Si}_{1-x}$ and ErSi_2 nanocrystals formed after high dose Ge and Er ion implantation in 4H-SiC, respectively, by HAADF-STEM tomography. Using continuous iterative reconstruction techniques, it was not only possible to visualize the nanoparticles with a diameter of 1-25 nm, but also erbium decorated voids and dislocation loops could be imaged in 3D. This allowed a detailed analysis of the shape and faceting of the particles as well as determination of the crystallographic orientation of the erbium decorated dislocation loops. These results will be compared to initial data obtained by discrete tomography.

In 2D, the nucleation, growth and structure of these clusters and nanocrystals have already been studied by Kaiser and coworkers using HRTEM and Z-contrast imaging [2-4]. Viewed along the [11-20] SiC projection, the ErSi_2 nanocrystals exhibit a characteristic hill-like shape with a well-defined flat base along the (0001) SiC basal plane [2]. Further faceting of these nanocrystals only becomes visible in 3D. We found that their basal plane typically exhibits strong hexagonal faceting corresponding to the $\{1-10\}$ class planes in SiC (Figure 1). Both their shape and orientation stay the same throughout most of the sample; only occasionally nanocrystals also exhibiting $\{11-2\}$ type facets are observed. Many of the nanocrystals are intersected by erbium decorated dislocation loops, which are typically oriented along the $\langle 1-100 \rangle$ direction in SiC (Figure 2).

In contrast, the overall shape of the $\text{Ge}_x\text{Si}_{1-x}$ particles is not as uniform as the ErSi_2 particles and the orientation varies significantly with respect to the SiC matrix. This variation of the 3D orientation confirms earlier calculations, which indicated several energy minima for a rotation of a $\text{Ge}_x\text{Si}_{1-x}$ crystal within a SiC matrix [3]. Nevertheless, for the first time, clear similarities between the shape of the ErSi_2 and $\text{Ge}_x\text{Si}_{1-x}$ could be observed. Together with the observed dislocations and voids, this could lead to a new dimension in interpretation of nucleation and growth of embedded nanocrystals.

References:

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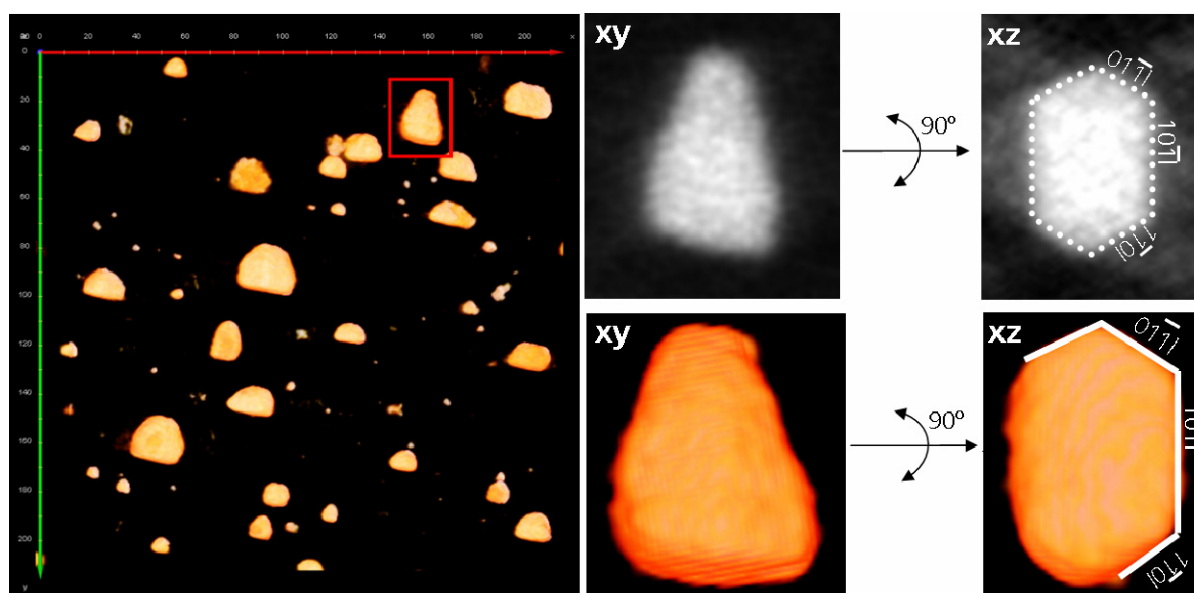


Figure 1: a) Volume rendering of ErSi_2 nanocrystals;
 b) Digital slices through the reconstructed volume of a selected ErSi_2 nanocrystal and volume rendering of that particle. The $\{01-11\}$ facets of the particle can be easily recognized in 3D.

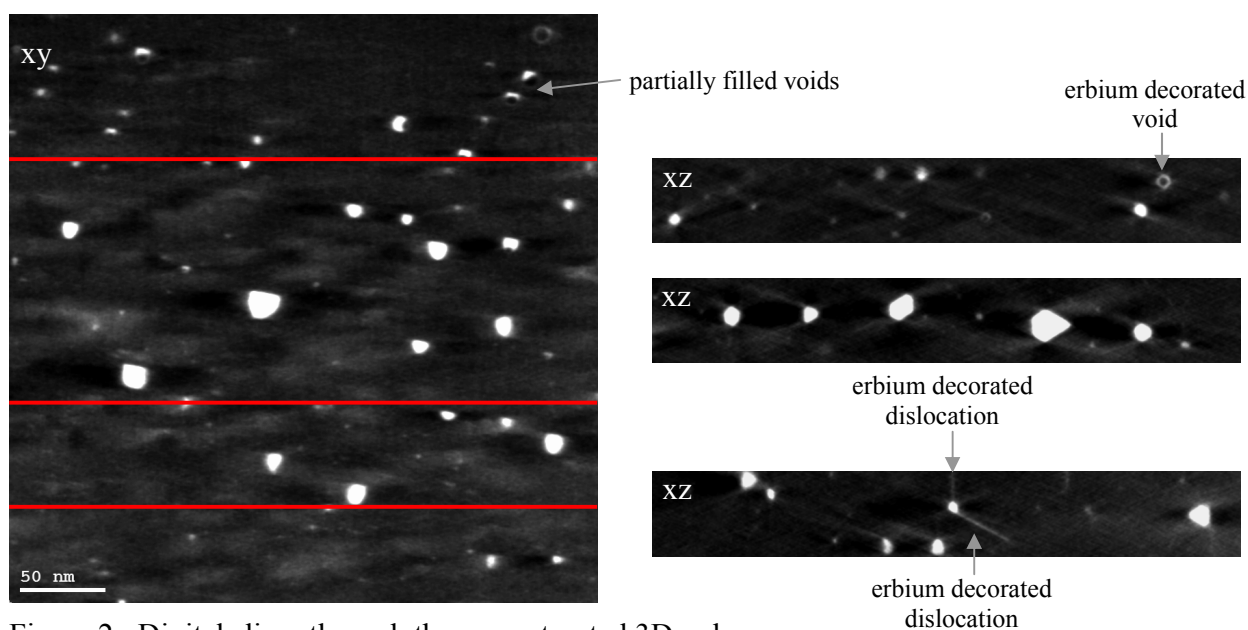


Figure 2: Digital slices through the reconstructed 3D volume
 a) In the XY plane, parallel to the 'normal' 2D view, nanocrystals and partially filled voids are visible.
 b) In the XZ plane erbium decorated voids and dislocation loops can be seen in addition to the faceting of the nanocrystals.