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Classification of artifacts in 3D-TEM tomography of FePt-MgO crystalline samples studied by multislice image simulation

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Size-controlled and well-arranged magnetic nano-granular materials are very important for development of future magnetic recording devices because they show new kinds of properties which have never been obtained in bulk magnets. High resolution electron microscopy has contributed so much to these kinds of research fields, but with its limitation of two-dimensional projected images of the samples. We have applied a three-dimensional (3D) electron tomography technique to FePt nanodots embedded in single crystalline magnesium oxide(MgO) films and succeeded in obtaining clear 3D images of the embedded dots with less than 1 nm image resolution, even though they are crystalline samples[1]. In order to interpret the successful result and study various kinds of origins to make artifacts on reconstructed 3D images, we have developed an image simulation routine for reconstruction of 3D images of those dots embedded in single crystalline films by using the multi-slice image simulation method and the 3D back-projection method.

FePt-MgO granular films were prepared by ultra-high vacuum deposition technique[2]. First, under a base-pressure of 6.7 x 10^{-6} Pa, MgO was deposited in 15 nm thickness using an electron heating source onto a cleaved NaCl (001) surface kept at 573 K. Then platinum(Pt), iron(Fe) and MgO (t=8nm) were deposited successively on the MgO film at 673 K. Pt and Fe were evaporated from another electron beam heating source and a resistance heating one, respectively. The average thicknesses of Pt and Fe were controlled to equiatomic ratio. After the deposition, sample was kept at 673 K for about 10 minutes, and the cooled gradually at a rate of 10-20 K/min. TEM observations were performed with a 300 kV TEM(TECNAI, F30) with a post-column energy filter(Gatan Imaging Filter), respectively. Image recording for 3D reconstruction was made on the TEM with an automated tilting recording system from –70 to + 70 degree with increment of 1 degree. 3D reconstruction was performed by using IMOD software and 3D visualization, by AMIRA software.

In the present study, a self-made simulation routine was developed for 3D image reconstruction of various structural models based on multislice image simulation software and IMOD. The calculation was made two-dimensionally corresponding to one-axial sample rotation in the present TEM. An FePt particle embedded in MgO single crystalline films was modeled by using a super-cell including tilt of the MgO crystals as illustrated in Fig. 1(a). The calculated image intensity was presented as many thin slabs corresponding to the tilt angles indicated in the right hand side in Fig. 1(b). Fig 2 shows an example of simulated 3D image in a two-dimensional space, which shows artifacts due to the missing cone effect, moiré-fringe effect and Fresnel fringe effect. In the present study, we are, for the first time, succeeded in clarifying artifacts of 3D image of crystalline samples such as the present FePt particles embedded in single

crystalline MgO films. Based on the results, we have successfully reconstructed 3D images as surface rendering images of Pt single crystalline catalytic clusters having double structured channels, which were prepared by using MCM-48 and previously observed by ADF-STEM tomography[3].

References

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[4] The present authors acknowledge Prof. O. Terasaki and Prof. R. Ryoo for giving Pt cluster samples. The present study was partly supported by grants from Japanese government as “Development of 3D electron microscope” and “Nano-hetero granular metals and their application”

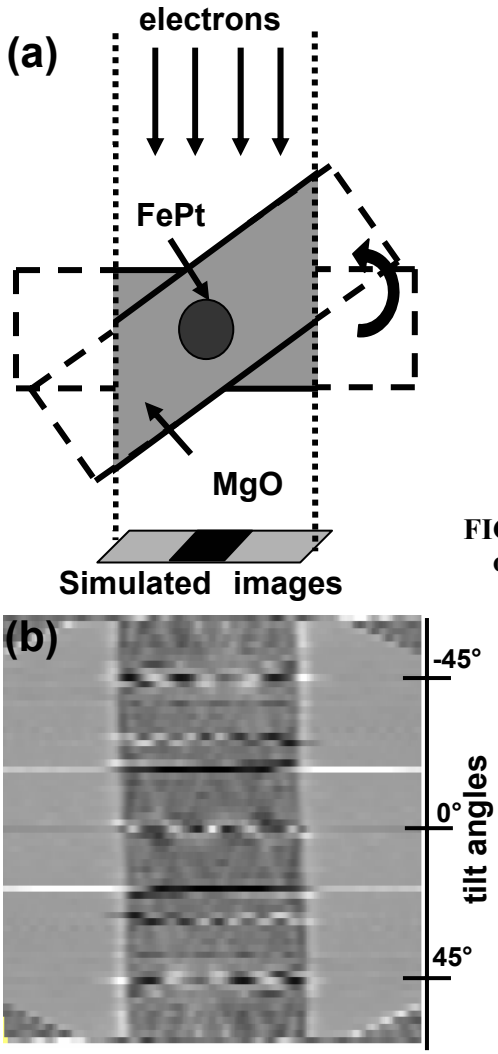

FIG. 1: (a)Illustration of a supercell for an FePt particle in MgO for multislice simulation, (b)Stack of slabs of calculated images corresponding to tilt angles.

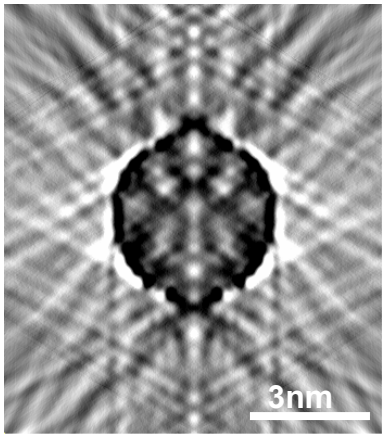

FIG. 2: Simulation of reconstructed image of an FePt particle two-dimensionally.

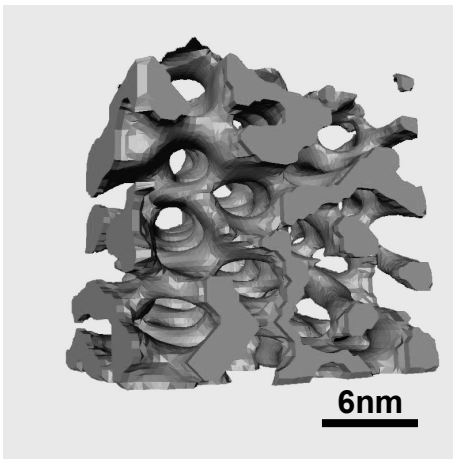

FIG. 3: Surface-rendering image of a Pt cluster molded in MCM-48.

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