GISAXS Analysis of Nanodots Extended into the Soft X-Ray Region

Grazing Incidence Small-Angle X-ray Scattering (GISAXS) measurements on Ge nanodots grown on Si (001) substrates and capped with an Si layer have been performed to explore the modeling and detailed analysis of three-dimensional structures buried in thin films in the hard (8.2 keV) and soft X-ray (1.8 keV) regions. Successful application of anomalous GISAXS at the K absorption edge of Si suggests that the present approach might be readily used for slightly harder photon energies, such as the K absorption edges of P and S.

Grazing Incidence Small-angle X-ray Scattering (GISAXS) is a useful tool to examine three-dimensional nanostructures in heterostructured thin films. To apply the method to light elements such as Si-based materials as well as soft matter containing phosphous and sulfur, etc., the use of anomalous scattering in the soft X-ray region is an attractive approach. GISAXS measurements in the soft X-ray region, however, may suffer from strong absorption by target materials and also from the q-range available at the wavelength. To explore technical solutions and analysis methods, GISAXS intensity for a model Ge nanodot sample has been analyzed both with conventional hard X-rays and also with soft X-rays at the K absorption edge of Si.

Ge nanodot samples grown on Si (001) substrates and capped with an Si layer by MBE or gas source MBE were used in the present experiments. GISAXS measurements with hard X-rays and cross-sectional TEM images demonstrated that the shape and size of the buried nanodots can be reconstructed by fitting two-dimensional GISAXS intensity in a kinematic framework [1]. Therefore, Distorted Wave Born Approximation (DWBA) simulations based on the three-dimensional shape of nanodots [1] and the layer structure obtained from least-squares fitting of reflectivity [2] were performed. DWBA simulations with hard X-rays confirmed the Born Approximation for shape analysis [2].

Figure 1 shows the measured and simulated GISAXS profiles of the same nanodot sample examined for shape analysis described above, obtained for the incident photon energy of 1.77 keV, where the K absorption edge of Si is at 1.839 keV [3]. As shown in Table 1, the refractive index of Si decreased sharply at 1.83 keV compared with that at 1.77 keV, thereby enhancing the contrast between Ge and Si at the edge. The intensity simulation with DWBA, taking the roughness and thickness of the layers obtained from the reflectivity measurements using Cu Kα radiation into account, reproduced the measured GISAXS profiles whose origin is Ge nanodots.

Table 1 Refractive indices of Si (left) and Ge (right) for the present experimental conditions

Energy	8.2 keV		1.83 keV		1.77 keV	
Material	Si	Ge	Si	Ge	Si	Ge
$\delta*10^5$	0.7	1.4	8	27	11	28
$\beta*10^6$	0.2	0.4	4	94	4	106

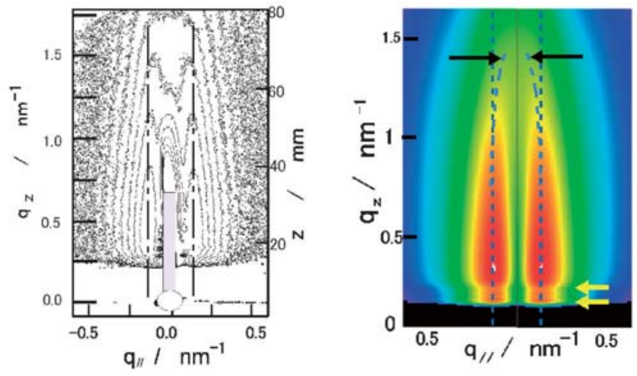

Figure 1
Measured (left) and simulated (right) GISAXS patterns of Ge nanodots capped with Si at 1.77 keV. Simulation was made with DWBA using layer structure parameters obtained from reflectivity data.

Enhancement of the scattering intensity at 1.83 keV with respect to that at 1.77 keV was confirmed [3]. Bending of interparticle interference towards smaller $q_{//}$ at large q_z due to the curvature of the Ewald sphere can be detected in the soft X-ray region, which is seen in the measured as well as simulated GISAXS pattern in Fig. 1. On the other hand, a strong diffuse scattering component at $q_{//} = 0$ in the measured pattern, attributed to the surface and interface roughness scattering, is not explained by the present simulation. An extended model that includes the simultaneous scattering process at the interface and also three-dimensional scattering body (GISAXS) is now being studied for further application of GISAXS in the soft X-ray region, where the surface itself may have both random or self-affine roughness and correlated replica undulation originated from the interior distribution of scattering bodies at the same time. This extension will be important for application to samples containing both film/membrane structures and nanoparticle objects.

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