Evolution of Kr precipitates in Kr-implanted Al as observed by the channelling method†

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It was discovered that heavy inert gases (Ar, Kr, and Xe) implanted into metals at room temperature precipitate in bubbles into a solid phase (solid precipitates) in the high-pressure state. It became possible to produce inert gas solids at room temperature by a rather simple technique, *i.e.*, ion implantation, without applying a high-pressure technique, and transmission electron microscopy (TEM) became feasible. Since then, the structure of inert gas solids, which are the simplest atomic solids, and the process from nucleation to formation of inert gas solids have been extensively studied mainly by TEM. TEM is very useful for investigating visible-sized bubbles and a lot of data on their structure and behaviour have been obtained. For invisible small-sized defects such as those in the initial stage of nucleation, channelling analysis is particularly useful, because it can provide direct information on the lattice location of implanted atoms.

In this study, processes from nucleation to formation of solid Kr precipitates in Al implanted with Kr atoms at room temperature are discussed. In previous studies, experiments were performed for four different implantation doses, 1, 4, 10×10^{14}, and 1×10^{16} Kr/cm^2, by the channelling method and/or TEM. By the channelling method, it was suggested that at low implantation doses, Kr atoms interact strongly with vacancies introduced during Kr-implantation to form various types of Kr-vacancy (V) complexes and they act as nucleation centres for the Kr precipitates. According to the TEM, at a dose of 1×10^{15} Kr/cm^2, a number of cavities were observed, while, at a dose of 1×10^{16} Kr/cm^2, the presence of epitaxially aligned fcc solid Kr precipitates with a 1.3 times larger lattice parameter than that of Al was observed. Between the stages of nucleation and formation of solid Kr precipitates, the initial stage of growth of Kr precipitates to bubbles and a key process towards the epitaxial alignment of solid Kr precipitates remain unclear. The objectives of this study are to elucidate such unresolved processes through a change in the site occupancy of Kr atoms with dose and to discuss the evolution of Kr precipitates from nucleation to formation of solid Kr precipitates. Therefore, the channelling experiment is extended to the specimens implanted with four higher doses from 2×10^{15} to 8×10^{15} Kr/cm^2 at intervals of 2×10^{15} Kr/cm^2.

Kr-implantation was carried out at room temperature at 50 keV into Al single crystal slices. Channelling angular scan was performed at room temperature by Rutherford backscattering spectroscopy (RBS) with a He^+ beam of 1.02 MeV accelerated by a tandem accelerator.

In the range of dose up to 2×10^{15} Kr/cm^2, Kr atoms are distributed over substitutional (S), tetrahedral (T), octahedral (O), and random (R) sites. With increasing dose, the fractions of T and S site occupancies decrease, while those of O and R sites increase. The T and O site occupancies are a result of the formation of Kr-V complexes; a Kr atom traps four vacancies (KrV_4) or six vacancies (KrV_6) to take configuration similar to trivacancy or pentavacancy, and is displaced to a T or an O site, respectively. The R site occupancy is attributed to Kr atoms associated with larger vacancy clusters. At low implantation doses, a Kr atom interacts with vacancies in its vicinity in the displacement cascade produced by the implantation of the Kr atom itself, because the overlapping of cascades is not significant. Such Kr-V complexes act as nucleation centres for the growth to Kr precipitates. With increasing dose, the overlapping of cascades becomes significant. In the initial stage of growth of Kr precipitates, not only existing Kr atoms at S sites but also additionally implanted Kr atoms migrate to Kr-V complexes, especially Kr associated large vacancy clusters, to be trapped, being assisted by mobile vacancies created by additional implantation (radiation-enhanced diffusion of Kr atoms). Thus, the fraction of Kr atoms associated with large vacancy clusters increases, resulting in Kr bubbles, which are in the fluid state. The fraction of the T site occupancy also decreases, while that of the O site occupancy increases.

At doses higher than 2×10^{15} Kr/cm^2, the fraction of the T site occupancy disappears, and that of the O site occupancy decreases. Instead, the displaced O (dis-O) site occupancy newly appears. This is interpreted as follows: small clusters of Kr atoms located at O and dis-O sites, the latter of which are displaced from O sites by about 0.4 Å in the ⟨112⟩ or ⟨110⟩ direction, are formed on the planes parallel to {111} planes at the bubble-matrix interface. They are precursors for the two dimensional growth of Kr layers in parallel to {111} planes with ordered arrangement of Kr atoms in the layers at higher implantation doses. With increasing dose to 8×10^{15} Kr/cm^2, bubbles, in which the pressure reaches the threshold value for solidification, solidify into an epitaxially aligned fcc structure. The ordered Kr layers act as a trigger for the formation of epitaxially aligned solid Kr precipitates. In the solidification, the increase in the internal pressure of bubbles by absorbing interstitials introduced during Kr implantation is important, as reported in previous channelling studies.[1)]

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Reference

1) E. Yagi, Phys. Rev. Lett. **67**, 3804 (1991).