Phonon Density of States in *fcc*-Fe Precipitates in Cu

Since a nuclear resonant scattering method gives us information only from the resonant nuclei, if we apply this method to the precipitates of a resonant nucleus, *e.g.* ^{57}Fe, we can obtain information for the Fe-precipitates alone, apart from the host metal. Accordingly, we can study how the host metal affects and how far the effect extends to the precipitates through the interface. Nano-particle precipitates have attracted widespread attention due to their many technological applications, such as improving the mechanical properties of materials. Therefore the data obtained provide important knowledge and can contribute to the development of new materials. In this article, we report the phonon density of states (DOS) of *fcc*-^{57}Fe precipitates in a Cu matrix, investigated using the nuclear resonant inelastic scattering method at beamline **BL09XU** [1].

Even below room temperature, Fe precipitates in Cu retain the *fcc* structure, which is stable for bulk crystal of Fe above 1185 K under normal atmospheric conditions. The precipitates are known to be spherical and are coherent with the Cu matrix, as shown in Fig. 1. The sizes of the precipitates can be easily controlled by thermal treatment [2]. The particle sizes of the precipitates with diameters of 3, 8, 15, 30, 50 and 80 nm were studied at room temperature. Experimental phonon DOSs determined from the present experiment for the *fcc*-Fe precipitates at various particle sizes are given in Fig. 2. The experimental data on the isolated Fe impurities in Cu previously reported by M. Seto *et al.* are also given as zero-nm precipitates for comparison [3]. With increasing particle sizes, phonon DOS curves show continuous change up to 15 nm, but no appreciable change is found above 30 nm, indicating that the influence of the Cu host extends to about 30 nm. Since all precipitates have a common atomic mass, these changes in the phonon DOS should be attributed to the inter-atomic forces $f_{Fe\text{-}Cu}$ and $f_{Fe\text{-}Fe}$. If the $f_{Fe\text{-}Cu}$ is greatly different from the $f_{Fe\text{-}Fe}$, the phonon DOS curves for small precipitates should be composed of two parts, one from the interface area ($f_{Fe\text{-}Cu}$) and

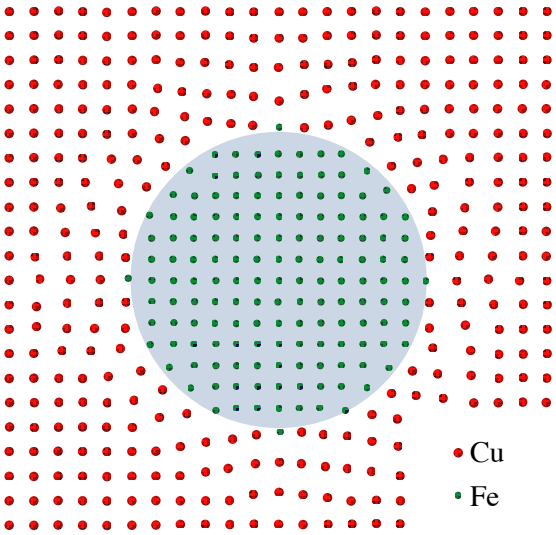

Fig. 1. Schematic illustration of coherent precipitates.

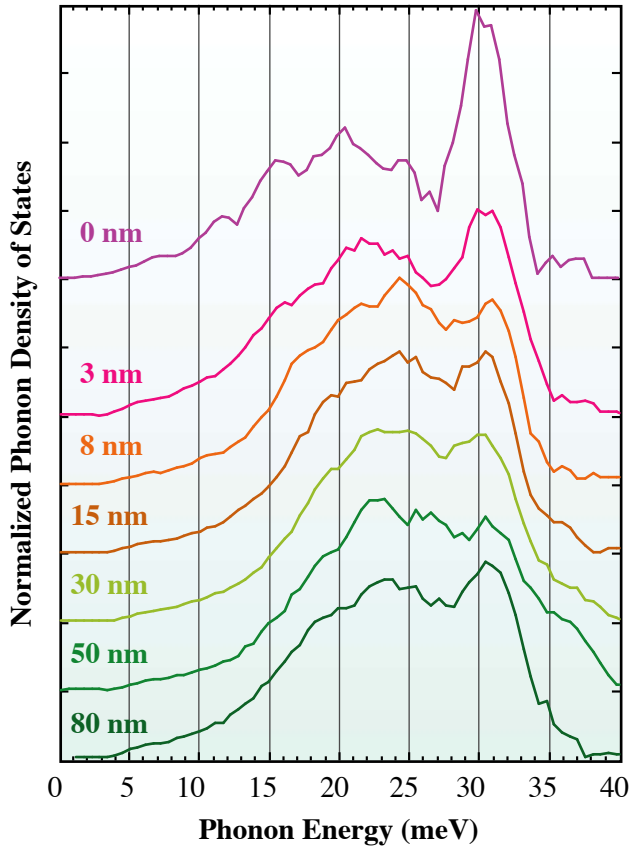

Fig. 2. Experimental phonon density of states (DOS) for various sizes of fcc-Fe precipitates in Cu measured at room temperature. Data for 0 nm indicate those for the isolated Fe impurities in Cu.

the other from inside the precipitates ($f_{Fe\text{-}Fe}$). The experimental phonon DOS changes gradually with increasing particle size. Thus, the influence of the Cu host is not confined to the interface area but uniformly extends over entire particles, and the effect should be attributed to the inter-atomic force $f_{Fe\text{-}Fe}$ itself. One possible explanation would be a change of the lattice parameter. The lattice parameter of the *fcc* -Fe precipitates is slightly smaller (0.7%) than that of Cu matrix and the precipitates are exposed to a strong expansive force. Consequently, the small precipitates have larger lattice spacing than the large ones [4], resulting in a change in the inter-atomic force $f_{Fe\text{-}Fe}$ of small precipitates.

Fcc -Fe precipitates in Cu undergo a structural phase transition at low temperature ($T_C \approx 65$ K), below which atomic positions are described by a periodic displacement wave propagating along the [1 1 0] direction with the <1 −1 0> polarization vector. Drastic softening of the sound velocity toward T_C has been reported [5]. Thus, the temperature variation of the phonon DOS for the *fcc* -Fe precipitates was also studied. Data obtained at various temperatures using the precipitates with a 50-nm diameter are given in Fig. 3. Phonon DOS curves show drastic change with decreasing temperature even though the displacement of lattices below T_C is very small. The peak intensity around 30 meV increases and the peak around 22 meV shifts toward the high-energy side with decreasing intensity. The structural phase transition is the first order, while

the change in phonon DOS appears to be continuous. The shape of the phonon DOS curve at 150 K already differs from that at room temperature, suggesting that the phonon dispersion curve, *i.e.*, inter-atomic potential starts to change far above the transition temperature. Recalling that *fcc*-Fe bulk crystal is stable only at much high temperature under normal atmospheric condition, we believe that the structural phase transition is the *fcc*-*bcc* martensitic transformation of the Fe metal. However, volume expansion and external shape change of the precipitates are tightly restricted by the host metal, and the martensitic transformation stopped at the halfway point of the transformation [6].

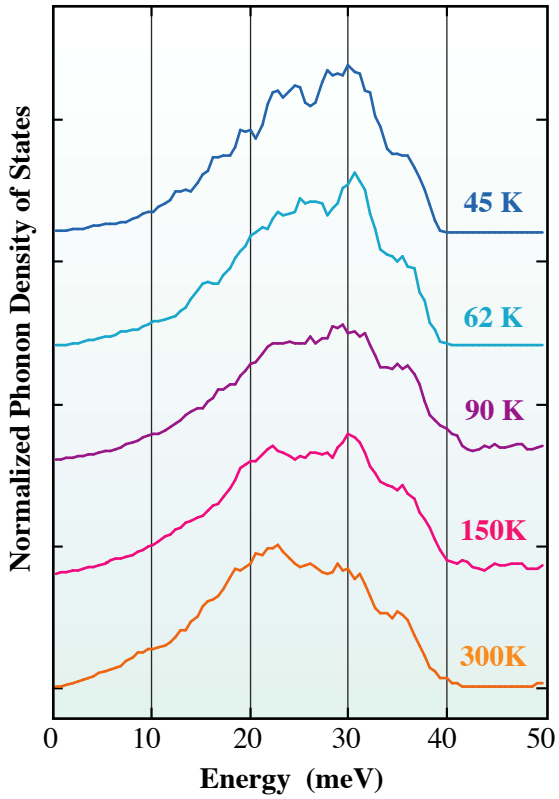

Fig. 3. Temperature variation of phonon density of states (DOS) of fcc-Fe precipitates. A specimen with precipitates of 50 nm in diameter was used.

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References

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