## LOCAL VIBRATIONAL DENSITIES OF STATES OF DILUTE Fe ATOMS IN METALS

The introduction of impurity atoms into an otherwise homogenous material is known to change its electronic, thermal and some other properties. The observation of the intrinsic vibrational densities of states of impurity atoms has been very difficult, particularly, in highly dilute impurity cases. The recent use of nuclear resonant inelastic scattering of synchrotron radiation, however, has made possible the direct observation of such states [1].

We have observed the local vibrational densities of states of $^{57}$Fe in Al–0.017 at.% $^{57}$Fe and Cu–0.1 at.% $^{57}$Fe foils [2]. In Fig. 1, obtained nuclear resonant inelastic scattering spectra are shown.

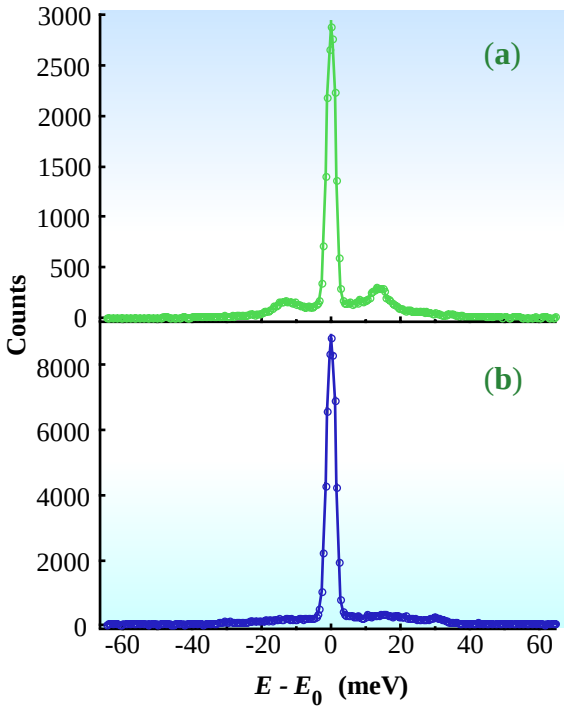


*Fig. 1. Nuclear resonant inelastic scattering spectra of synchrotron radiation by $^{57}$Fe in **(a)** Al-0.017 at.% Fe and **(b)** Cu-0.1 at.% Fe.*

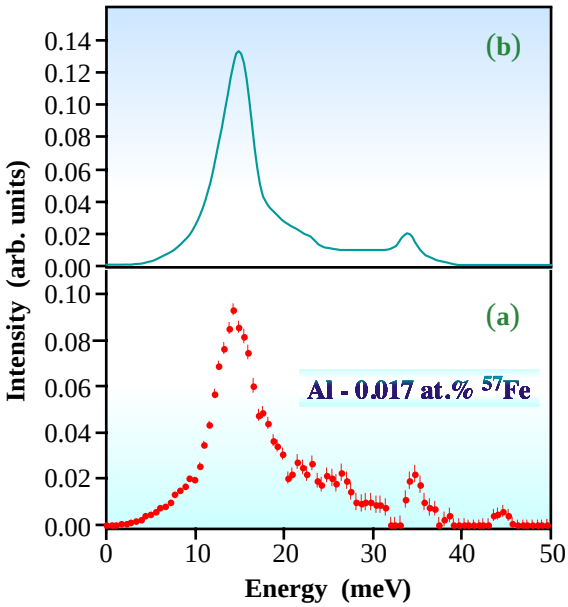


*Fig. 2. **(a)** Vibrational density of states of $^{57}$Fe in Al-0.017 at.%. **(b)** Response function of the impurity Fe atom to the phonon density of states of Al metal.*

From the measured spectra, the vibrational densities of states of $^{57}$Fe in Al–0.017 at.% $^{57}$Fe and Cu–0.1 at.% $^{57}$Fe were obtained (Figs. 2(a) and 3(a), respectively). The obtained spectra are different from those of host (metals) [3,4]. For the analysis of the obtained results, we adopted the Green's function technique developed by Mannheim *et al*. [5,6]. This theory has only one adjustable parameter – an effective force constant . It enables one to calculate vibrational densities of states of the dilute substitutional Fe atom in Al and Cu using the unperturbed phonon densities of states of Al [3] and Cu [4]. Calculated results are shown in Figs. 2(b) and 3(b), respectively. In general, the theory implies the existence of resonance modes, whose frequencies lie in the range of the normal modes of the unperturbed host crystal. Furthermore, in the case that the mass of an impurity atom is sufficiently light and/or the binding of an impurity atom to the host crystal is sufficiently stiff, the theory shows that there may

be a localized mode, whose frequency is greater than the maximum frequency of the unperturbed crystal. The measured spectrum of Fe in Al shows the resonant vibration modes superimposed upon host Al vibrational modes. In the measured spectrum of Fe in Cu, the peak interpreted as a localized mode is found just above the phonon cut-off energy (30.6 meV) of Cu metal. The existence of such a peak was predicted but has not yet been confirmed [7]. In general, the measurement of the local vibrational densities of states have demonstrated high reproducibility.

The results show the latest developments and progress in this area of research. In the future, we have a plan to study the local vibrational densities of states systematically of $^{57}$Fe and $^{119}$Sn atoms in various metals and semiconductors.

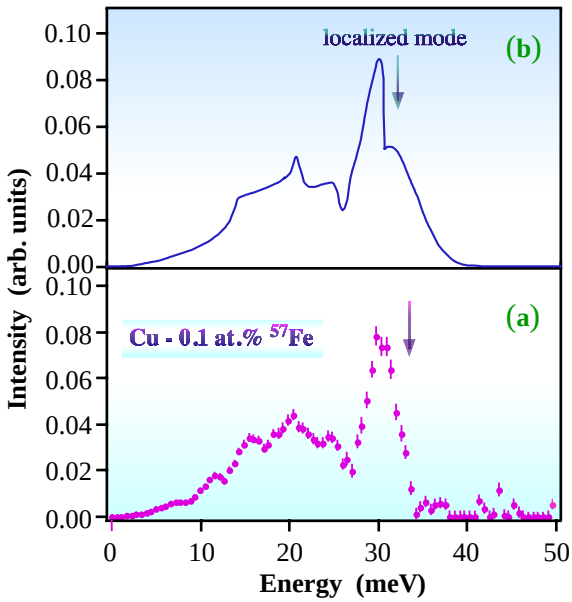


*Fig. 3.* ***(a)*** *Vibrational density of states of $^{57}$Fe in Cu-0.1 at.%.* ***(b)*** *Response function of the impurity Fe atom to the phonon density of states of Cu metal.*

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**References**

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