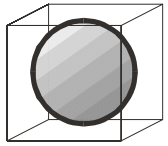
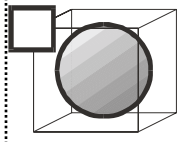
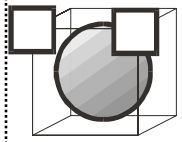
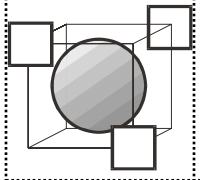
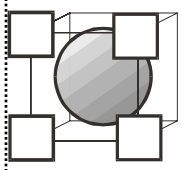
A hierarchy of vacancy complexes observed in FeAl

Perturbed angular correlation spectroscopy has the ability to resolve different local environments of probe atoms.

This is illustrated from a recent study of thermal defects in FeAl, an intermetallic compound having the simple CsCl structure [1]. The table at right, adapted from the paper, shows different configurations of a solute atom having from 0 to 4 near neighbor lattice vacancies.

One configuration was observed for each n-order complex. Comparison of observed quadrupole interaction frequencies with predicted ones is good.

Complex	Predicted frequency	Observed frequency	Ratio
	0	0	0
	1	141	(1)
	1.76	278	1.97
	1	181	1.28
	0	70	0.50

[1] *Point defects in FeAl studied by perturbed angular correlation*, Gary S. Collins, Luke S.-J. Peng and Matthew O. Zacate, Defect and Diffusion Forum 213-215, 107-132 (2003).

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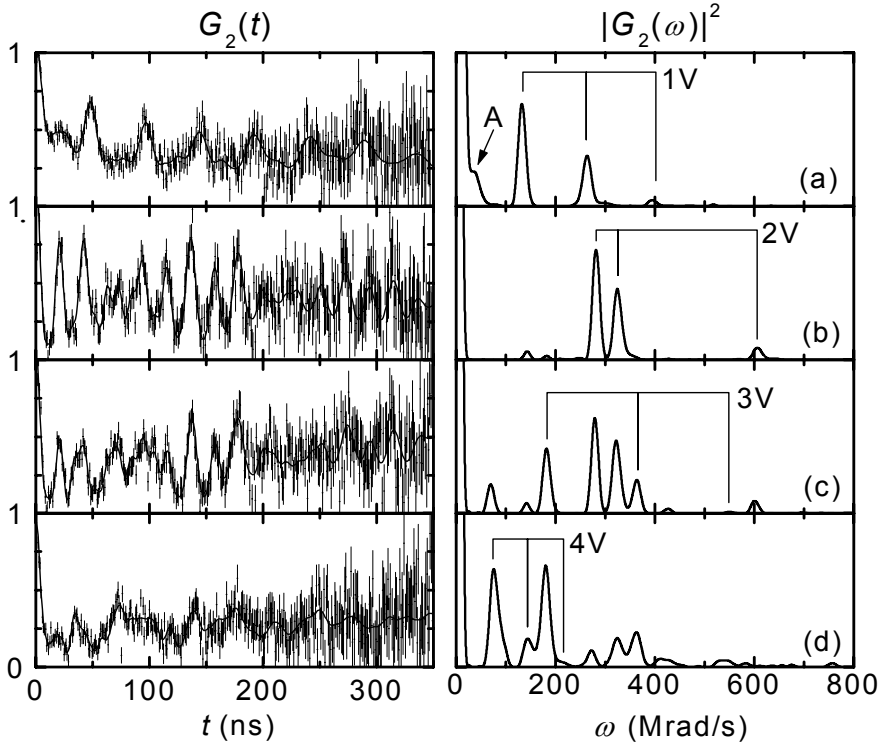
In the figure are PAC spectra exhibiting most clearly the signals for complexes with 1, 2, 3 and 4 vacancies. Each signal has three frequency harmonics shown in the fourier transforms on the right.

Identification of signals with underlying complexes was made using calculations of electric field gradients (previous page) and simulations of changes in site fractions of signals observed in measurements made at different temperatures (next page).



PAC spectra made for indium impurity probes in FeAl containing excess vacancies on the Fe-sublattice.

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The site fractions were observed to change reversibly as a function of the temperature of measurement, due to "condensation" and "evaporation" of the excess vacancies. The figure shows observed changes for samples having five different compositions, together with simulated changes assuming that signals are identified as shown.

Agreement between experiment and simulation can be seen to be excellent. Only using PAC has one been able to observe such detailed defect reactions between vacancies and solute atoms.

End.