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# A new first principles approach to calculate phonon spectra of disordered alloys

Oscar Grånäs<sup>1</sup>, Biswanath Dutta<sup>2</sup>, Subhradip Ghosh<sup>2</sup> and Biplab Sanyal<sup>1</sup>

<sup>1</sup> Department of Physics and Astronomy, Uppsala University, Box-516, SE-75120 Uppsala, Sweden

<sup>2</sup> Department of Physics, Indian Institute of Technology Guwahati, Guwahati-781039, India

E-mail: [biplab.sanyal@physics.uu.se](mailto:biplab.sanyal@physics.uu.se)

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## Abstract

The lattice dynamics in substitutional disordered alloys with constituents having large size differences is driven by strong disorder in masses, inter-atomic force constants and local environments. In this paper, a new first principles approach based on special quasirandom structures and an itinerant coherent potential approximation to compute the phonon spectra of such alloys is proposed and applied to Ni<sub>0.5</sub>Pt<sub>0.5</sub> alloy. The agreement between our results and experiments is found to be much better than for previous models of disorder due to an accurate treatment of the interplay of inter-atomic forces among various pairs of chemical species. This new formalism serves as a potential solution to the longstanding problem of a proper microscopic understanding of lattice dynamical behavior of disordered alloys.

(Some figures may appear in colour only in the online journal)

The energy dispersion of lattice waves in ordered inter-metallics and disordered alloys has recently gained significant importance due to its role in stabilizing a particular structural phase by contributing toward the system's entropy and in pinpointing the fundamental mechanism behind the behavior of materials, which are important in technological applications. Examples include the connection between martensitic transformations in shape-memory alloys and the anomalous behavior of their phonon spectra [1], the anomalously low thermal-expansion coefficients in Fe-based Invar alloys and the unusual behavior of the phonon frequencies under external pressure [2], and the dramatic alteration of relative stabilities of different precipitates in the Al–Cu system due to vibrational entropy [3].

Theoretical investigation on lattice dynamics in disordered metallic alloys is one of the most challenging areas in state of the art materials science research. Mostly theoretical studies have been carried out on the alloy compounds although a wealth of neutron-scattering data is available for various disordered alloys with arbitrary compositions. The dearth of theoretical works is due to the lack of a suitable self-consistent, analytical methodology to carry out the

averaging over the random configurations, taking into account the disorder due to the fluctuations in mass, force constant and local environment around an atom. The most widely used method is the single-site coherent potential approximation (SCPA) [4], which, being a single-site theory, is unable to handle the non-local fluctuations. The recently developed itinerant coherent potential approximation (ICPA) [5] is a successful generalization of the SCPA for handling disordered alloys with large mass as well as force constant disorder. While the ICPA stands as a self-consistent, analytic, site-translational invariant tool for computing the phonon spectra in disordered alloys, a missing key component in establishing it as an accurate and reliable formalism is its integration with a tractable structural model for positional disorder which can closely mimic the fluctuations in the inter-atomic force constants in a random alloy. Moreover, due to the presence of short-range order, the phonon spectra of such systems would be affected by the dominant vibrations of unlike species pairs. Initially, attempts were made in the form of first principles computation of inter-atomic force constants from selected ordered structures and then these were used in a random alloy environment [6, 7]. This is not a proper remedy

as the force constants are not directly transferable across the environments [8, 9].

In this paper, we present a new first principles based formalism to compute the lattice dynamics of substitutional disordered alloys which incorporates the effects of disorder in mass, force constant and environment. We demonstrate the formalism by computing the phonon dispersion spectra of  $\text{Ni}_{0.5}\text{Pt}_{0.5}$  alloy. This alloy is chosen as its constituents have large mass differences (Pt being three times heavier than Ni), large size differences ( $\sim 11\%$ ) and large force constant differences (the Pt–Pt force constants being  $\sim 55\%$  larger than the Ni–Ni ones) and thus significant effects of all three kinds of disorder on the lattice dynamics can be expected. Also, neutron-scattering experiments [10] show anomalous features in the dispersion curves in the form of resonance modes and splitting of the dispersion branches. In previous works, neither SCPA [10] nor ICPA [5] with an empirical set of force constants has achieved good quantitative agreement with experiments, signifying that the inter-atomic interactions have not been modeled accurately.

Our formalism has three important steps: first we generate a structural model of substitutional disorder by the special quasirandom structure (SQS) method, then averaging of the force constant tensor is carried out to recover the original symmetry of the solid solution, followed by the ICPA for performing the averaging over configurations.

- (i) *Structural model.* First principles supercell calculations of disordered alloys involve the direct averaging of the properties obtained from a number of disordered configurations of the alloy. Current computational capabilities limit the size of the supercell necessary to describe each configuration, as well as the number of configurations sampled. Zunger *et al* developed a computationally tractable approach to model the disorder through the introduction of the SQS method [11], an  $N$ -atom per cell periodic structure designed so that their distinct correlation functions  $\Pi_{k,m}$  best match the ensemble-averaged correlation functions  $\langle\langle\Pi_{k,m}\rangle\rangle$  of the random alloy. Here  $(k, m)$  corresponds to the figure defined by the number  $k$  of atoms located on its vertices ( $k = 2, 3, 4, \dots$ , are pairs, triangles, tetrahedra, etc) with  $m$  being the order of neighbor distances separating them ( $m = 1, 2, \dots$ , are first, second neighbors, etc). As properties like the equilibrium volume, local density of states and bond lengths around an atom are influenced by the local environment, SQS forms an adequate approximation. The biggest advantage of the SQS over a conventional supercell to model positional disorder is that the former uses the knowledge of the pair-correlation functions, a key property of random alloys, to decide the positions of the atoms in the unit cell, instead of inserting them randomly as is done in the conventional supercell technique, and thus it is guaranteed to provide a better description of the environments in an actual random alloy.
- (ii) *Averaging procedure.* The force constant tensors between a given pair of atoms calculated using the SQS will have

nontrivial off-diagonal elements due to low symmetry. Moreover, due to the atomic relaxations in a local environment, a distribution of bond distances for a pair of species gives rise to a distribution in their force constants. To extract the force constant tensors having the symmetry of the underlying crystal structure of the disordered alloy, we average the calculated SQS force constant matrices for a particular set of displacements of the atoms from their ideal positions in the lattice, related by symmetry that will transform the force constant matrices to one displaying the symmetry of the underlying crystal structure. These averaged force constant tensors are then used as the inputs to the ICPA for the calculation of the configuration-averaged quantities. Below, we demonstrate the idea for an FCC lattice.

In an FCC lattice, the distances between a given atom and its 12 nearest neighbors are specified by the vectors  $(\pm\frac{1}{2}, \pm\frac{1}{2}, 0)a$ ,  $(\pm\frac{1}{2}, 0, \pm\frac{1}{2})a$  and  $(0, \pm\frac{1}{2}, \pm\frac{1}{2})a$ ,  $a$  being the lattice parameter. The force constant matrix for two atoms separated by the vector  $(\frac{1}{2}, \frac{1}{2}, 0)a$  is of the form

$$\begin{pmatrix} A & B & 0 \\ B & A & 0 \\ 0 & 0 & C \end{pmatrix}.$$

The other nearest neighbor force constant matrices are of the same form and are related by point group operations. However, when the atoms are allowed to relax, the vector separating a pair of nearest neighbor atoms is modified to  $(\frac{1}{2} \pm \delta_1, \frac{1}{2} \pm \delta_2, \delta_3)a$  and the matrix of force constants corresponding to a given pair of atoms reflects the loss of symmetry, taking the general form

$$\Phi = \begin{pmatrix} a_1 & b_1 & a_3 \\ b_2 & a_2 & a_4 \\ a_6 & a_5 & c \end{pmatrix}. \quad (1)$$

For a particular set of  $\delta_1$ ,  $\delta_2$  and  $\delta_3$ , one needs to perform the averaging such that we obtain the following force constant matrix:

$$\Phi' = \begin{pmatrix} a' & b' & 0 \\ b' & a' & 0 \\ 0 & 0 & c' \end{pmatrix}. \quad (2)$$

To achieve this, one needs to pick up the relevant ones out of the 48 symmetry operations corresponding to the cubic group which transform the force constant matrices to one displaying the symmetry of the FCC structure. To elaborate on this, we provide the following example.

Suppose, two atoms are separated by the separation vector  $\vec{R} = \{\frac{1}{2} - \delta_1, -(\frac{1}{2} + \delta_2), -\delta_3\}a$ . The force constant matrix obtained from first principles calculations on the SQS is given by equation (1). To recover the symmetry of the FCC force constants, we need to find out the transformations that transform the separation vector  $\vec{R}$  to new separation vectors  $\vec{R}' = \{\frac{1}{2} - \delta_1, \frac{1}{2} + \delta_2, -\delta_3\}a$  and  $\{\frac{1}{2} + \delta_2, \frac{1}{2} - \delta_1, -\delta_3\}a$ . These transformations, in this

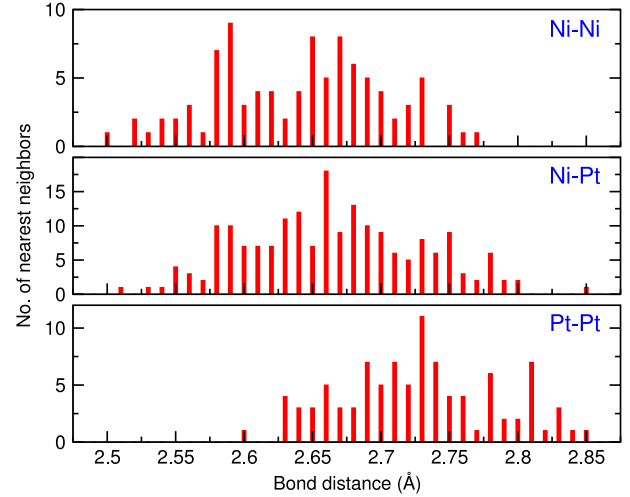
particular case, mimic the nearest neighbor separation  $(\frac{1}{2}, \frac{1}{2}, 0)a$  for the unrelaxed FCC lattice. They are

$$\begin{aligned} (x, y, z) &\longrightarrow (y, -x, z) \\ (x, y, z) &\longrightarrow (x, -y, z) \\ (x, y, z) &\longrightarrow (y, -x, -z) \\ (x, y, z) &\longrightarrow (x, -y, -z). \end{aligned} \quad (3)$$

Corresponding to each of these transformation, there is a transformation matrix  $U$ . We transform the SQS force constant matrix  $\Phi$  to the FCC force constant matrix  $\Phi'$  by performing the operation  $U^T \Phi U$  in each of the four cases and then adding them. This simple procedure produces  $a' = 2(a_1 + a_2)$ ,  $b' = -2(b_1 + b_2)$  and  $c' = 4c$ . All other off-diagonal elements vanish due to this symmetrization and the FCC symmetry is recovered. This procedure is repeated for all pairs of force constants and an arithmetic average is finally computed.

- (iii) *The ICPA.* The ICPA is a Green's function based formalism that generalizes the SCPA by considering scattering from more than one site embedded in an effective medium within which the effect of this correlated disorder is built in. The medium is constructed in a self-consistent way so that site-translational invariance and analyticity of the Green's function are ensured. The analyticity of the Green's function is ensured by using the principles of the traveling cluster approximation [12] which showed that once there are non-diagonal terms in the Green's function, the self-energy must include iteration of the scatterer through the sample to preserve analyticity. This means that the physical observables would be site translationally invariant. This required translational invariance is ensured by expressing the operators associated with the physical observables in an extended Hilbert space which accounts for the statistical fluctuations in the site occupancies due to disorder.

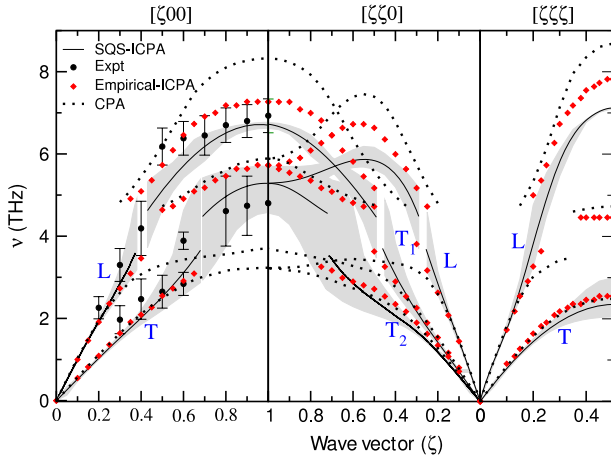
We employ the first principles plane wave projector augmented wave method within the generalized gradient approximation (GGA) [13] as implemented in the VASP code [14] for the calculation of the Hellman–Feynman forces on the atoms in a 64-atom SQS cell ( $4 \times 4 \times 4$  supercell of the primitive FCC unit cell) with the optimized lattice parameter of 3.93 Å. Our value of the lattice parameter is slightly larger than the experimental value of 3.78 Å due to the use of the GGA. The SQS generated structure has zero short-range order in the first four neighboring shells indicating a homogeneous disorder. The cut-off energy for the electronic wavefunctions is 400 eV. 432  $k$ -points were used in the irreducible Brillouin zone for the calculations of the force constant matrix. We have tested the convergence of our results with respect to the relevant parameters and have concluded that our choice yields quite accurate results. To obtain the force constant matrix, first, the equilibrium geometry is obtained by relaxing the atomic positions in the SQS cell until the forces converge to  $10^{-4}$  eV Å<sup>-1</sup>. Then each atom in the SQS cell is moved by 0.01 Å from the equilibrium position along three Cartesian



**Figure 1.** Dispersion of bond distances for three pairs of atoms computed by the SQS.

axes and the forces on the atoms are calculated. Due to the lack of any symmetry in the SQS cell, 64 different force constant matrices are generated by using the PHON code [15]. The symmetry averaging procedure is then used to obtain an effective  $3 \times 3$  force constant matrix to be used in the ICPA calculation. In the ICPA, the disorder is considered in the nearest neighbor shell only as the further neighbor force constants are one order of magnitude less. The ICPA calculations are made with a  $25 \times 25 \times 25$   $k$ -mesh and 1000 energy points.

In figure 1, the variations of the number of nearest neighbors of a given type are plotted as a function of the bond distances. It is observed that the inter-atomic bond distances depend sensitively on the number of unlike atoms, which clearly proves the dependence of the bond distances on the local environment. As a result of this, the inter-atomic force constants also undergo variations. The calculated average Ni–Ni ( $d_{\text{Ni–Ni}}$ ), Ni–Pt ( $d_{\text{Ni–Pt}}$ ) and Pt–Pt ( $d_{\text{Pt–Pt}}$ ) bond distances are 2.64 Å, 2.66 Å and 2.73 Å respectively, indicating a significant dispersion among the three pairs of bonds. A comparison with the unrelaxed alloy bond distances reveals that the relaxed  $d_{\text{Ni–Pt}}$  remains the same,  $d_{\text{Ni–Ni}}$  is less than 1% smaller and  $d_{\text{Pt–Pt}}$  is 2.6% larger. The force constants for three different models of disorder, namely, SQS-averaged, empirical [5] and SCPA are presented in table 1. In [5], it was argued that the Ni–Ni bonds in the alloy are softer compared to those in pure Ni, the Pt–Pt bonds are stiffer compared to those in pure Pt and the Ni–Pt bonds are even softer than the Ni–Ni ones because the Ni–Pt bond distances were thought to be the largest. A comparison between the force constants obtained by the SQS-averaged and this empirical scheme shows that the Ni–Ni force constants computed by the SQS-averaging scheme are 50% softer, and the Ni–Pt and Pt–Pt force constants are 25% and 23% harder on average. More importantly, the Ni–Pt force constants computed by the SQS-averaging scheme are harder than the Ni–Ni ones, a result in contradiction with the empirical scheme. This difference occurs due to the proper inclusion of environmental



**Figure 2.** Phonon dispersion in  $\text{Ni}_{0.5}\text{Pt}_{0.5}$  alloy computed by SQS-ICPA (solid line), SCPA (dotted line) and empirical-ICPA [5] (red diamonds). The circles indicate the experimental results. The shaded regions indicate the disorder-induced widths calculated by the SQS-ICPA.

**Table 1.** Real-space nearest neighbor force constants  $\Phi_{ss'}^{\alpha\beta}$  (in  $\text{dyn cm}^{-1}$ ) for  $\text{Ni}_{50}\text{Pt}_{50}$  obtained by averaging the SQS force constants, the force constant matrix  $\Phi^{\alpha\beta}$  used for SCPA calculations and the empirical force constants [5]. The final column indicates the Cartesian components of  $\Phi^{\alpha\beta}$ .

Pair	SQS	SCPA	Empirical	$\alpha\beta$
Ni–Ni	–8 231	–19 365	–15 587	$xx$
Ni–Pt	–17 868	–19 365	–13 855	$xx$
Pt–Pt	–33 494	–19 365	–28 993	$xx$
Ni–Ni	525	3 255	436	$zz$
Ni–Pt	2 820	3 255	348	$zz$
Pt–Pt	6 854	3 255	7 040	$zz$
Ni–Ni	–9 580	–22 679	–19 100	$xy$
Ni–Pt	–20 740	–22 679	–15 280	$xy$
Pt–Pt	–39 655	–22 679	–30 317	$xy$

disorder in our case.  $d_{\text{Ni–Ni}}$  in the alloy as computed by the SQS is about 6% larger than in pure Ni and thus these bonds suffer the most severe dilution in strength,  $d_{\text{Pt–Pt}}$  reduces by about 1% compared to that in pure Pt and thus these bonds are harder by about only 15% compared to those in pure Pt. In spite of nearly the same bond distances, the Ni–Pt bonds computed by the SQS are stiffer than the Ni–Ni bonds for the following reasons: in case of the Ni–Pt pairs, the Ni atoms find much larger Pt atoms as their nearest neighbors, with roughly the same available space as they have in the case of Ni–Ni pairs. As a result, the smaller Ni atoms try to accommodate larger Pt atoms within the same volume as that available for Ni–Ni pairs, resulting in a hardening of the Ni–Pt nearest neighbor interactions compared to the Ni–Ni ones.

In figure 2, we present the phonon dispersion curves of  $\text{Ni}_{0.5}\text{Pt}_{0.5}$  alloy computed using the force constants obtained by the three models of disorder. The configuration averaging in the cases of the SQS and the empirical schemes is carried out using the ICPA. SQS-ICPA shows the best agreement with experiments as compared with the SCPA and the empirical-ICPA [5]. The disorder-induced widths

computed by the SQS-ICPA method (the shaded region in figure 2) also agree reasonably well with experiments. The comparisons with experiments were possible only for the  $[\zeta 00]$  direction because experimental results were not available for other directions. A closer look at figure 2 reveals that for the low-frequency branches, the empirical-ICPA and SQS-ICPA methods are in close agreement while there are significant differences for the high-frequency branches. The mass-disorder treated in SCPA, on the other hand, fails to reproduce the experimental features of the dispersion relations both qualitatively and quantitatively. The frequencies of the high-frequency branches (both transverse and longitudinal) computed by the SCPA are severely overestimated while the lower frequency branches extend all the way to the zone boundary, thus displaying a split-band behavior in the phonon dispersions which is not observed experimentally.

All these observations can be understood in terms of the inter-atomic force constants (shown in table 1) which are influenced by the fluctuations in the local environment. In the SCPA, the fluctuations in the force constants are completely neglected and hence Ni–Ni, Ni–Pt and Pt–Pt all have the same force constants. In earlier studies [10, 5], the force constants used in the SCPA were those of pure Ni obtained experimentally [16]. In this study we have used a more realistic set of force constants for the SCPA calculations which are  $\Phi^{\alpha\beta} = x^2 \Phi_{\text{Ni–Ni}}^{\alpha\beta} + (1-x)^2 \Phi_{\text{Pt–Pt}}^{\alpha\beta} + 2x(1-x) \Phi_{\text{Ni–Pt}}^{\alpha\beta}$ , where  $\alpha, \beta$  are the Cartesian directions and  $x$  is the concentration of Ni.  $\Phi_{ss'}^{\alpha\beta}$  are the SQS-averaged force constants where  $s, s'$  denote atomic species. Such a choice of force constants has been used to incorporate, in an average way, the effects of alloy environment. The results, nevertheless, suggest that unless the fluctuations in the force constants are incorporated, the results do not even agree qualitatively with the measurements. The frequencies of the upper (lower) branches of the longitudinal and transverse modes computed by the SCPA are too high (low) as compared with experiments. Ni–Ni vibrations dominate the higher frequency branches and, as the average force constants are too high, the frequencies are pushed away from the ones measured by neutron-scattering, while the lower frequency branches, being solely due to the Pt–Pt vibrations, have lower frequencies due to the underestimation of the Pt–Pt force constants. The empirical-ICPA results on the other hand agree qualitatively with experiments because there is no split-band like behavior as was seen in the SCPA. This is due to the consideration of the Ni–Pt correlated vibrations which renormalize the spectral weights associated with the contributions from Ni–Ni and Pt–Pt pairs [5]. Moreover, the splitting of the vibrational branches, found experimentally around  $\zeta = 0.55$  as a signature of the existence of a resonance mode, is reproduced and the frequencies of the high-frequency branches are better as compared to the SCPA. The Ni–Ni (Pt–Pt) force constants shown in table 1 in the empirical model are softer (harder) as compared to the SCPA ones, explaining the reason for the better agreement of the phonon frequencies computed by the empirical-ICPA model with the experimental results. However, the overestimation (underestimation) of the Ni–Ni



(Pt–Pt) interactions and an incorrect qualitative estimation of the Ni–Pt interactions as compared to the Ni–Ni ones gives rise to significant discrepancies for the high-frequency longitudinal and transverse branches. With the SQS–ICPA, one can have a much better quantitative agreement between theory and experiments, as seen in figure 2. The high-frequency branches for both longitudinal and transverse vibrations computed by the SQS–ICPA method agree substantially with the experimental results. The normal mode frequencies for these branches are dominated by the vibrations of the Ni pairs and thus a softening of the Ni–Ni bonds as computed by the SQS pushes the frequencies downwards compared to the empirical model making a better agreement with experiments. Similarly, the relaxations of the Pt atoms result in stiffening of the Pt–Pt bonds, thus pushing the frequencies slightly upwards. However, the high-frequency transverse branch computed by the SQS–ICPA model is still overestimated. In neutron-scattering measurements [10], there were some ambiguities in determining the peak positions of the line shapes for the high-frequency transverse modes and thus the experimental results for this branch had larger uncertainties. Given this fact, the agreement between the theory and the experiment can be considered to be fairly good.

In conclusion, we have developed a reliable first principles based approach for the calculation of phonon spectra in substitutional disordered alloys to treat mass, force constant and environmental disorder on an equal footing. We demonstrate in the case of Ni<sub>0.5</sub>Pt<sub>0.5</sub> alloy the importance of an accurate structural model of disorder taking into account the role of fluctuations in the local environment through atomic relaxations in interpreting the microscopic features of the lattice dynamics for this class of complex alloy. The accurate modeling of the environmental disorder made possible by the SQS paves the way for a reliable description of phonon spectra in alloys with short-range order where the force constants between a pair of species are dominated by a particular configuration of the nearest neighbor environment around an atom. Our future aim is to calculate the thermodynamic quantities [17] to compare with experiments. Finally, we conclude that a combination of

reliable force constants obtained from *ab initio* and ICPA as a self-consistent analytic method for configuration averaging enables us to solve the longstanding problem of theoretical computation of lattice dynamics in disordered alloys.

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