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Short Communication: Symmetry-correct bonding in density functional theory calculations for delta phase Pu

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Abstract

The long-held conclusion that magnetic order in delta phase Pu makes the structure mechanically unstable in density functional theory calculations is incorrect if the magnetic order is allowed to be non-collinear. The non-collinear 3Q spin structure is intrinsically cubic and makes all structurally equivalent bonds equivalent in their bonding character. Applied to density functional theory calculations on delta phase Pu, the 3Q spin structure results in elastic constants and phonons with the correct symmetry. The calculated phonon dispersion agrees better with experiment than previous calculations, and the calculated thermal expansion shows the unique behavior seen experimentally: it is negative.

Advances toward a better understanding of plutonium continue after many decades of research. The driver for the advances is two-fold: the nature of the $5f$ electrons, and the effects due to the material's self-irradiation. The challenging nature of the $5f$ electrons stems from Pu demarcating the boundary between the early actinides with itinerant $5f$ electrons and the late actinides with localized $5f$ electrons [1]. Self-irradiation continuously

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introduces lattice imperfections that affect the phase stabilities of Pu-based materials [2], including the face-centered cubic (fcc) crystal structure of the δ -Pu phase, whose temperature range of stability, 315-450 °C [3], can be expanded to include room temperature by doping with Ga and other elements [4]. The lattice imperfections, be they from doping or from self-irradiation, change the thermal properties; these effects need to be understood if they are to be controlled. For this to be successful, the first challenge must be further addressed.

Even the high-symmetry delta phase of Pu remains incompletely understood. In particular, aspects of δ -Pu related to magnetism remain unlike the behavior of conventional magnetic materials. Density functional theory (DFT) calculations with spin polarization have advanced to where many of the material's remarkable and unusual facets are well described [5, 6, 7, 8, 9]. This approach has its critics since magnetic moments are not observed as in conventional magnetic materials [10]. Recent experiments indicate a fluctuating spin structure [11], which underpins DFT calculations in which a special quasi-random spin structure models the magnetic disorder and is interpreted as a static snapshot of the fluctuations [8].

The introduction of disordered spin structures also serves to overcome the mechanical instabilities caused by ordered spin structures [8, 9, 12, 13]. In particular, the AFM spin structure is the lowest-energy spin structure and is frequently used in calculations. To date it has been assumed that any magnetic order in δ -Pu is mechanically unstable [8, 9].

The work here shows that this assumption is incorrect if the spin structure is allowed to be non-collinear. The non-collinear 3Q spin structure identified

in γ Fe-Mn alloys by Umebayashi and Ishikawa [14] is intrinsically cubic. With it, all equivalent bonds in the fcc structure become equivalent in their bonding character, and the delta phase of Pu is mechanically stable. The 3Q spin structure generalizes the antiferromagnetic (AFM) spin structure; comparisons of results from the two spin structures are made below. Comparisons with experiment show improved results for the 3Q spin structure, but these comparisons are an imperfect gauge: experimentally, δ -Pu is a high-temperature phase and not stable at low temperatures.

Results presented here stem from calculations performed with DFT as implemented in the VASP package [15, 16]. The electronic states are treated with the projector augmented wave method [17], in the generalized gradient approximation of Perdew, Burke, and Ernzerhof [18], with first-order Methfessel-Paxton smearing (width 0.2 eV) [19], and a cutoff energy for the plane wave basis set of 500 eV. The k-point mesh density is well converged; specifically, the elastic constant calculations on the four-atom conventional unit cell use a $12 \times 12 \times 12$ mesh, and the phonon calculations on the 64-atom supercell ($4 \times 4 \times 4$ primitive unit cells) use a $6 \times 6 \times 6$ mesh. Spin-orbit coupling is included in all calculations. Orbital polarization is not included, though it is key to getting the correct equilibrium volume [9].

Phonons are calculated with the small-displacement method [20, 21, 22]. One atom in the computational cells is displaced in all symmetry-inequivalent Cartesian directions, and the forces calculated with DFT serve to construct the force constants. These are used to construct the dynamical matrix for wave vectors \mathbf{q} , and diagonalization delivers the phonon frequencies at each \mathbf{q} . The elastic constants are calculated analogously: the computational cell

is strained along individual and pairs of Cartesian directions, and the stresses calculated with DFT serve to construct the elastic constants.

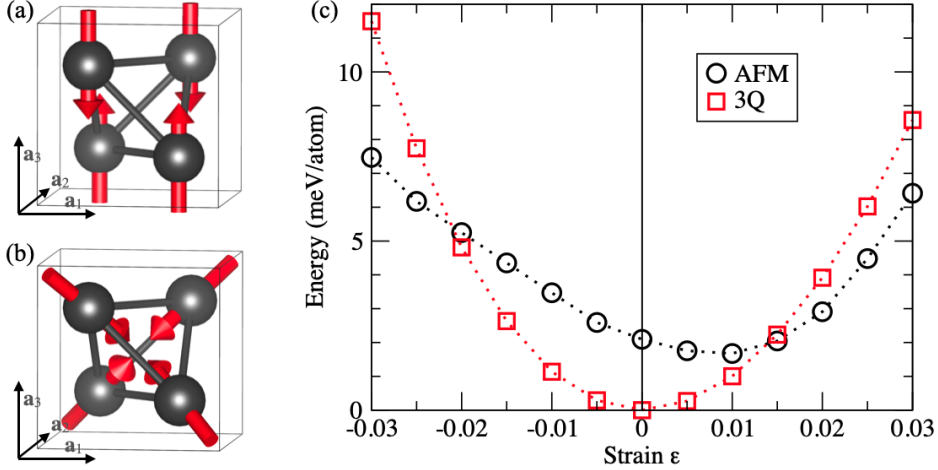


Figure 1: Conventional four-atom fcc unit cell with (a) AFM and (b) 3Q spin structures and (c) the calculated energy plotted as a function of applied tetragonal strain at fixed volume (24.97 \AA^3). The calculations employ the four-atom conventional unit cell and use a $16 \times 16 \times 16$ k-point mesh.

The mechanical instability due to the AFM spin structure relates directly to structurally equivalent bonds differing in their bonding character [9]. Fig. 1(a) shows the AFM spin structure, whose alignment along the lattice parameter a_3 breaks the cubic symmetry. For the AFM spin structure, Fig. 1(c) shows the calculated energy at fixed volume is minimized by a tetragonal strain of approximately $\epsilon = +0.01$. This strain increases the lattice parameters a_1 and a_2 by 1% and decreases a_3 by almost 2%. Referring to bonds between atoms with the same spin as “FM bonds” and bonds between atoms with opposite spins as “AFM bonds,” the FM bonds lengthen, and the

AFM bonds shorten. These changes correlate with the pressures calculated for the corresponding spin structure: the pressure for the FM spin structure (all FM bonds) is positive, the pressure for the AFM spin structure (2/3 AFM bonds, 1/3 FM bonds) is negative.

Fig. 1(b) shows the non-collinear 3Q spin structure in which all structurally equivalent bonds are equivalent in their bonding character. The 3Q spin structure is the linear combination of the AFM spin structures oriented along the x , y , and z Cartesian coordinates. Whereas the AFM spin structure flips the spin polarization between nearest-neighbor atoms along one Cartesian direction, the 3Q spin structure flips two Cartesian components of the spin polarization between all nearest-neighbor atoms (leaving the third Cartesian component unchanged). This move from AFM to 3Q retains the 2/3 AFM and 1/3 FM character of the bonding, but this 2 : 1 distribution changes from global over all bonds to local within each bond. For the 3Q spin structure, Fig. 1(c) shows the energy is minimized by zero tetragonal strain: with the 3Q spin structure δ -Pu is mechanically stable in DFT calculations.

The DFT calculations in Fig. 1(c) show the energies of the 3Q and AFM spin structures are nearly equivalent. While these calculations with VASP show the 3Q having slightly lower energy, similar calculations with the all-electron code Elk [23] reverse the order. The difference between AFM and 3Q energies, which is very sensitive to the applied smearing, will be explored elsewhere.

	C_{11}	C_{22}	C_{33}	C_{12}	C_{13}	C_{23}	C_{44}	C_{55}	C_{66}
AFM	53.92	54.02	36.04	37.15	34.88	34.80	32.48	32.18	32.88
3Q	50.10	50.09	50.13	33.94	33.95	33.95	34.80	34.81	34.83
experiment	36.28			26.73			33.59		

Table 1: Elastic constants calculated for δ -Pu at $a = 4.64 \text{ \AA}$, given in units of GPa. The excessive precision is chosen to show how closely calculations with the 3Q spin structure respect the cubic symmetry in which $C_{11} = C_{22} = C_{33}$, $C_{12} = C_{13} = C_{23}$, and $C_{44} = C_{55} = C_{66}$. The experimental values [24] are given for reference, they are measured on samples that necessarily contain lattice defects due to the self-irradiation. Furthermore, the experimental values are measured at room temperature on a δ -Pu sample stabilized with 1 wt. % Ga, while the calculated values are for pure δ -Pu at 0 K.

The change from inequivalent to equivalent bonding similarly affects the elastic constants, as shown in Tab. 1. The AFM spin structure has to be aligned along one Cartesian direction, chosen here to be parallel to the lattice parameter a_3 , which breaks the cubic symmetry, seen most clearly in $C_{33} \neq C_{11} = C_{22}$. For the intrinsically cubic 3Q spin structure, the stress-strain responses retain the cubic symmetry to high precision. The values of the elastic constants remain, in general, stiffer than the experimental values. This difference is likely due to the effects of lattice imperfections, which are present in measurements but not in these calculations, the effects of temperature, which is 300 K for the measurements and 0 K for the calculations, and the doping with 1 wt. % Ga of the experimental system.

The inherently cubic symmetry of the 3Q spin structure implies that the phonons also obey the symmetries imposed by the fcc crystal structure. Fig. 2 shows the calculated phonon dispersion agrees well with the experimental

data of Wong et al. [25]. The exception to this is at shorter wave lengths along the [111] direction, though the agreement is better than for previous theoretical results, as is the case for most of the dispersion. As with the elastic constants, the comparison is approximate, as the experimental data is measured at 300 K on a system stabilized with 2 wt. % Ga, while the calculations are for a pure Pu system at 0 K.

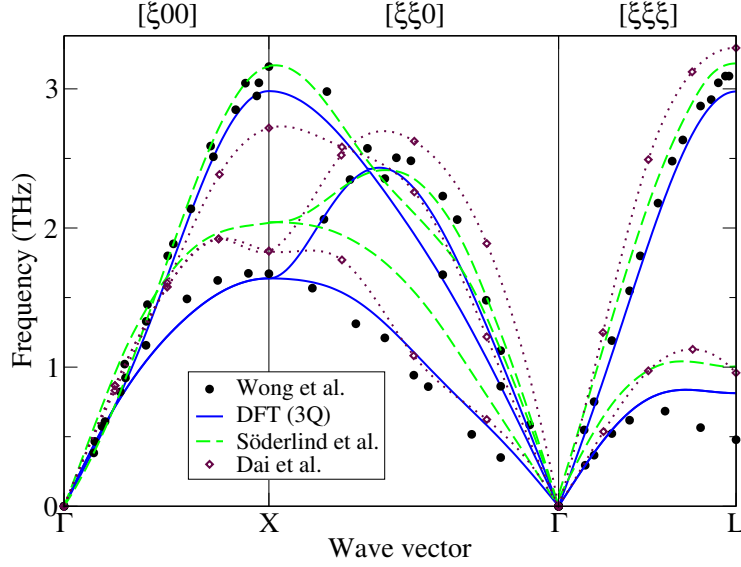


Figure 2: Phonon dispersion for δ -Pu at the experimental lattice constant (4.64 Å) calculated at 0 K with the 3Q spin structure. Circles represent the room temperature experimental data for δ -Pu stabilized with 2 wt. % Ga [25]. Previous theoretical results employing DFT at 0 K and 4.635 Å (Söderlind [9]) are represented by dashed green lines and results employing dynamical mean field theory (DMFT, Dai *et al.* [26]) are represented by maroon diamonds with dot-dashed lines to guide the eye.

Elastic constants and phonons that have the correct finite-temperature symmetries provide a reliable foundation for investigating Pu’s properties at

finite temperatures. The correct symmetries are well approximated in DFT calculations with a disordered spin structure, which more accurately represents the fluctuating spin structure indicated in experiment. Evidence for a corresponding symmetry breaking by the electrons appears in DFT+ U calculations, wherein a Hubbard correction U is added [27]. In this case, the fcc structure reveals unstable phonon modes at 0 K. From a practical point of view, however, there are advantages to a spin structure that has all appropriately equivalent bonds: calculations of, e.g., how a lattice imperfection affects thermal properties can be performed with a single atomic configuration. The same calculations with a disordered spin structure would require multiple configurations with the lattice imperfection sampling different local environments.

An example of δ -Pu's unique thermodynamic behavior is its thermal expansion, which is evaluated here with the quasi harmonic approximation. Based on the phonons calculated on a 40^3 mesh of wave vectors throughout the first Brillouin zone, the free energy is evaluated at a given volume for a sequence of temperatures. Repeating this procedure for a sequence of volumes and fitting the sequence of free energies for a specified temperature gives an isotherm with an equilibrium volume for that temperature. Within the DFT framework, the quasi harmonic approximation captures the anharmonicity, because the forces calculated in response to the displacement remain essentially unchanged with a doubling of the displacement's magnitude.

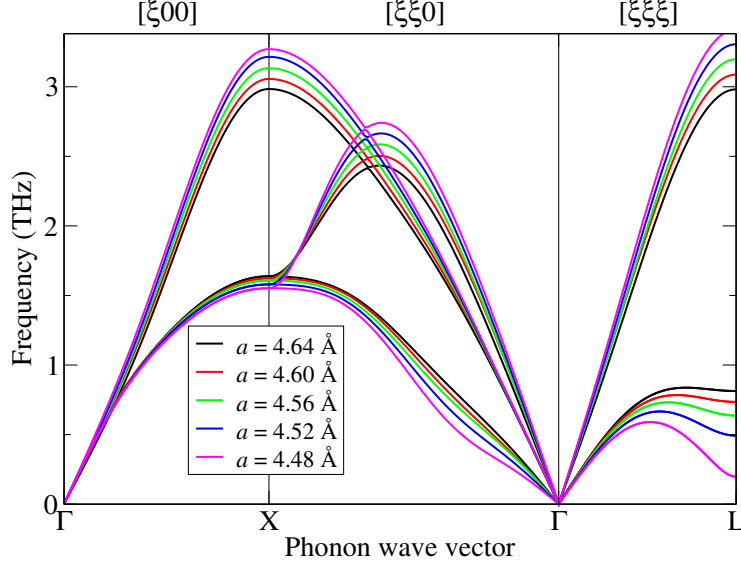


Figure 3: Phonon dispersion for δ -Pu at a sequence of lattice constants calculated with the 3Q spin structure.

Fig. 3 shows that changing the volume affects the phonons in a unique way. As the volume contracts toward the theoretical minimum at approximately $a = 4.52 \text{ \AA}$, the longitudinal modes stiffen as in most materials and as expected from the compression of the bonds. Both transverse modes along $[100]$ and $[111]$ and transverse mode one along $[110]$, however, soften. To the author's knowledge, no experiments have attempted to measure how volume influences the phonons of δ -Pu. A measurement of the influence of temperature shows no sign of softening of the transverse mode at L [28], albeit for a sample containing 0.6 wt. % Ga for which the thermal contraction is quite small [29]. (Also notable is how at smaller volumes the phonon dispersion starts to exhibit the kink along $[110]$ and the downward bending along $[111]$)

seen in experiment [25] but not in the present calculations at the experimental volume.)

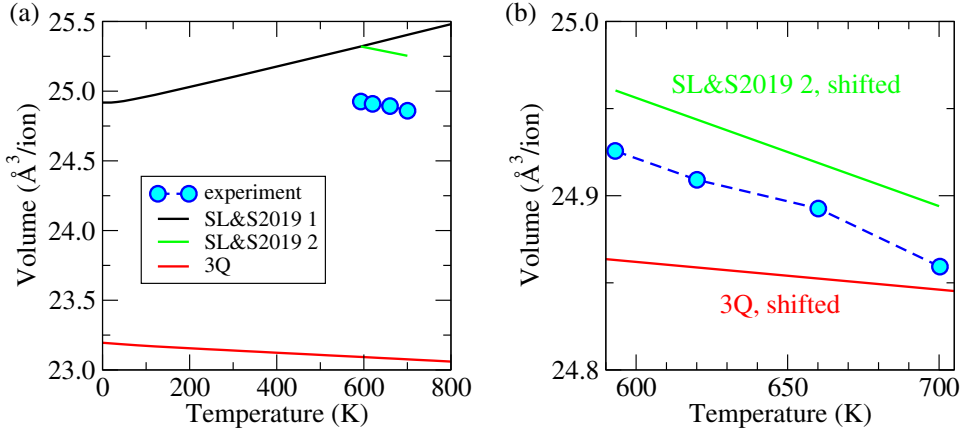


Figure 4: Thermal expansion of δ -Pu calculated with the 3Q spin structure in the quasi harmonic approximation. (a) The 3Q results give a volume that is too small compared to experiment [29, 30] and compared to previous theory [9], but the slope is negative unlike the results of a DebyeGrneisen model for the lattice vibrations (SL&S2019 1). (b) The 3Q result, shifted upward in volume for comparison, decreases about half as fast as experiment and the previous theory result (SL&S2019 2) that combines contributions from the lattice vibrations and spin fluctuations [9].

The unique changes to the phonons lead to a thermal expansion that is negative. The typical positive thermal expansion of most materials comes from the softening of the phonons with increasing volume. Lower frequencies enhance the entropic contribution of the phonons to the free energy, increasingly lowering the free energy with larger volumes. Fig. 4 compares the negative thermal expansion to experimental data [29, 30] and previous theoretical results [9]. In the latter, the thermal expansion calculated with

a disordered spin structure and a DebyeGrneisen model for the lattice vibrations is positive, but adding the effects of spin fluctuations produces a negative thermal expansion. The thermal expansion calculated here with the 3Q spin structure is negative, though with a lesser slope. The difference in the slope of the volume contraction shows the importance of including spin fluctuations. Additional influences on the slope can be expected from self-irradiation induced defects, which are present in experiment but not the calculations. Such defects result in local bonding structures that resemble the lower-volume phases of Pu [31] and may induce additional phonon modes that soften with contraction.

In summary, the observation that an ordered spin structure leads to mechanical instability in DFT calculations of delta phase Pu is correct, but only for collinear spins. The ordered, non-collinear, and intrinsically cubic 3Q spin structure introduced to δ -Pu here removes the mechanical instability. Elastic constants and phonons of δ -Pu calculated with DFT calculations and the 3Q spin structure show the correct symmetry, and the phonons agree with experiment better than previous DFT and DMFT calculations. Finally, the 3Q-DFT calculations show a unique stiffening of most transverse phonon modes at contracted volumes, which in turn leads to a calculated thermal expansion that is negative, as observed in experiment.

Data availability

The raw/processed data required to reproduce these findings may be made available by contacting the author depending on institutional require-

ments.

Declaration of competing interests

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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