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First-principles elastic constants and phonons of δ-Pu

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Elastic constants and zone-boundary phonons of δ-plutonium have been calculated within the density-functional theory. The paramagnetic state of δ-Pu is modeled by disordered magnetism utilizing either the disordered local moment or the special quasirandom structure techniques. The anomalously soft C' as well as a large anisotropy ratio (C_{44}/C') of δ-Pu is reproduced by this theoretical model. Also the recently measured phonons for δ-Pu compare relatively well with their theoretical counterpart at the zone boundaries.

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I. INTRODUCTION

The last few years have seen a remarkable focus on plutonium metal, both experimentally as well as theoretically. In addition to its importance as a nuclear power source, it has many anomalous properties that are challenging to explore and understand. Many aspects of Pu metal were recently reviewed by Hecker *et al.*,[1] which we refer to for a more general discussion. In the present paper we focus on the high symmetry, low density, and technologically important Pu phase, namely, δ-Pu. Although crystallized in a close-packed simple arrangement, face-centered cubic (fcc), this phase may be the most puzzling piece in the Pu puzzle. Experimentally, recent studies of δ-Pu include heat capacity, resistivity, susceptibility, photoemission, elasticity, and phonon dispersions. These measurements paint a complex picture of δ-Pu for which the theory that otherwise is suitable for metals is unable to account. Consequently, new theoretical models have been developed that try to link the many properties of δ-Pu, which sometimes seem contradicting. The key feature of these models have been to reproduce the anomalous atomic density of δ-Pu. Compared to the ground-state monoclinic α phase, the δ phase is stabilized at a 25% larger atomic volume at a modest temperature of 593 K. Elaborate density-functional calculations that are quite reasonable for α-Pu (Ref. 2) cannot account for this expansion. Other models, such as the mixed-level model (MLM),[3] can reproduce the expanded volume for δ-Pu, however. The MLM also has the advantage of being able to correctly describe the electronic structure when compared to photoemission data.[4] It is based on the idea that the $5f$ band in δ-Pu is split into two levels, one appropriate for a valence state (one $5f$ electron) and the other a nonbonding core state (four $5f$ electrons) with some hybridization allowed with the valence states. This approach seems to be unable to correctly describe any other phase, including the ground-state α phase, and is therefore of limited use for the understanding of many other facets of Pu.

Another rather successful model of δ-Pu is derived from the dynamical mean-field theory.[5,6] Here correlation effects are incorporated by means of an onsite Hubbard parameter "U," believed to be responsible for the expanded volume and other anomalous properties of δ-Pu. Indeed, this approach reproduces the correct atomic density when the Hubbard parameter U is chosen to be about 4 eV.[5] Recently this model produced elastic constants and phonons for δ-Pu that are in remarkable agreement with experiment.[6] Compared to the MLM, however, this technique is less accurate in producing an electronic structure that is consistent with the photoemission data.

The last model we discuss is most closely related to traditional density-functional theory (DFT), which has been proven to be so successful for many metallic systems including the light actinides.[7] It was discovered, by several researchers,[8–10] that allowing the magnetic spin to polarize reduces the $5f$ bonding in δ-Pu sufficiently to expand the lattice to an atomic density in very good agreement with experiment. The hypothetical zero temperature ground-state spin configuration for fcc Pu has been confirmed to be antiferromagnetic ($L1_0$ structure), whereas it has been proposed[11] that δ-Pu is paramagnetic (PM) (with substantial magnetic moments) which is well described by disordered magnetic moments. In addition to reproducing the anomalous lattice constant in δ-Pu, this approach offers (i) mechanical stability of δ-Pu, (ii) a mechanism that explains the δ-Pu$\rightarrow\gamma$-Pu transition, (iii) an electronic structure that is fully compatible with δ-Pu photoemission measurements.[11,12] The notion of magnetism in Pu is somewhat controversial and there has been no direct experimental evidence of magnetic moments in Pu. The magnetic susceptibility is largely temperature independent, although resistivity measurements may suggest existence of local magnetic

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moments.[1,13] The fact that δ-Pu, alloyed with americium (a nonmagnetic element), shows a Curie-Weiss behavior[13] of its magnetic susceptibility also lends support to this idea. In addition, it has been shown that when magnetic effects such as spin/orbital polarization and spin-orbit coupling are incorporated in the theory, virtually all known phases of Pu are well described.[14]

In the present study, we adopt the magnetic model of Pu and calculate bulk properties of δ-Pu including elastic constants and zone-boundary phonons which are compared to recent measurements. Section II deals with computational details of our electronic structure calculations, Sec. III provides a discussion of the results, and finally in Sec. IV we summarize.

II. COMPUTATIONAL DETAILS

In order to study δ-Pu we have applied three established electronic structure techniques similar to what has been done before.[11] Common for any DFT approach is the need for an assumption of the electron exchange and correlation functional. The generalized gradient approximation[15] has been successful for actinide metals in the past[7] and is used throughout this study.

Specific details regarding the exact muffin-tin orbitals (EMTO), full potential linear muffin-tin orbitals (FPLMTO), and the projected augmented plane-wave (PAW) calculations are presented below.

The calculations we have referred to as EMTO are performed using a scalar-relativistic, spin-polarized Green's function technique based on an improved *screened* Korringa-Kohn-Rostoker method, where the one-electron potential is represented by optimized overlapping muffin-tin (OOMT) potential spheres.[16–19] It is spherically symmetric inside and constant outside these spheres. The radii of the potential spheres, the spherical potentials inside them, and the constant value from the interstitial are determined by minimizing (a) the deviation between the exact and overlapping potentials and (b) the errors coming from the overlap between spheres. Thus, the OOMT potential ensures a more accurate description of the full potential compared to the conventional muffin-tin or nonoverlapping approach because it is optimized to best represent a nonspherical (full) potential.

Within the EMTO formalism, the one-electron states are calculated *exactly* for the OOMT potentials. As an output from the EMTO calculations, one can determine the self-consistent Green's function of the system and the complete, nonspherically symmetric, charge density. Finally, the total energy is calculated using the full charge-density technique.[19,20]

For the total energy of random substitutional alloys, the EMTO is combined with the coherent potential approximation[21] (CPA) that also allows for the treatment of magnetic disorder.[22,23] In the present work, as well as in our previous papers,[11,12,24,25] a PM δ-Pu was modeled within the DLM approximation.[26] This state uses a random mixture of two distinct magnetic states, namely, the spin-up and spin-down configurations of the same atomic species in a system.

The calculations are performed for a basis set including valence *spdf* orbitals and the semicore 6*p* state whereas the core states are recalculated at each iteration. Integration over the irreducible wedge of the fcc Brillouin zone (BZ) is performed using the special *k*-point method[27] with 916 *k* points. The Green's function has been calculated for 40 complex energy points distributed exponentially on a semicircle with a 1.9 Ry diameter enclosing the occupied states. The equilibrium density of δ-Pu is obtained from a Murnaghan fit[28] to about 15 total energies calculated as a function of lattice constant. For the calculation of C' and C_{44} we use volume conserving orthorhombic and monoclinic strains, respectively.[29] The zone-boundary (ZB) phonons are calculated similarly to what was done earlier.[30]

The parameters of the FPLMTO calculations are the same as those given previously,[10] but the more important details are repeated here. The approximations in this method are limited to the approximation of the exchange/correlation energy functional, cut offs in the expansion of basis functions, *k*-point sampling in integrations over the BZ, and the Born-Oppenheimer assumption. Spin-orbit coupling and spin/orbital polarization are accounted for, in the same way as have been described earlier.[10]

The use of full nonsphericity of the charge density and one-electron potential is essential for the calculation of small distortions. This is accomplished by expanding charge density and potential in cubic harmonics inside nonoverlapping muffin-tin spheres and in a Fourier series in the interstitial region. We use two energy tails associated with each basis orbital and for 6*s*, 6*p*, and the valence states (7*s*, 7*p*, 6*d*, and 5*f*) these pairs were different. With this "double basis" approach we use a total of six energy tail parameters and a total of 12 basis functions per atom. Spherical harmonic expansions are carried out through $l_{max}=6$ for the bases, potential, and charge density. Two types of crystal structures are considered here. First, the antiferromagnetic, ferromagnetic, and nonmagnetic configurations are accounted for in a two atom/cell simple tetragonal structure. Within this structure the axial c/a ratio distinguishes between fcc ($c/a=\sqrt{2}$) and body-centered cubic (bcc: $c/a=1$). Other c/a values are also considered when studying mechanical instabilities. The special quasirandom structure (SQS) model[31] with an eight atom (SQS8) supercell is used to approximate a disordered magnetic structure with zero total spin moment. The sampling of the irreducible BZ is done using the special *k*-point method[27] and the number of *k* points used were up to 240 in the two atom/cell calculation and about 60 for the eight atom/cell calculation. To each energy eigenvalue a Gaussian is associated with 20 mRy width to speed up convergency.

The PAW approach is an extension of the norm-conserving pseudopotential scheme,[32] which is a powerful technique for performing large-scale static as well as dynamic DFT calculations using a plane-wave basis set. Transferable pseudopotentials of this kind, however, can become computationally very expensive when applied to transition or *f*-electron systems, because of the required small core radius. A remedy to this problem was proposed by Vanderbilt in the ultrasoft pseudopotential scheme,[33] where the norm-conserving condition is relaxed and the core radius can be moved out to approximately half of the nearest-neighbor distance. In this approach, localized atom-centered augmentation charges need to be introduced. Blöchl[34] developed a

TABLE I. Calculated equilibrium volume (Å^3), bulk and elastic moduli (GPa), and zone-boundary phonons (THz) for δ-Pu. Magnetic configurations are denoted *D* for disordered, FM for ferromagnetic, and NM for nonmagnetic.

Method	V	B	C'	C_{44}	X_L	X_T	L_L	L_T
EMTO (*D*)	25.5	38	8.1	81	7.5	2.7	2.9	1.3
PAW (*D*)	23.9	46	10	30	3.0	1.3	2.5	1.3
FPLMTO (*D*)	24.9	41	18	48				
FPLMTO (FM)	25.6	26	17	27	2.9	1.9	2.3	0.63
FPLMTO (NM)	17.8	165	−69	15				
Experiment	25.0,[a,b]	30[a], 29[b]	4.8[a], 4.9[b]	34[a], 31[b]	3.1[b]	1.7[b]	3.1[b]	0.48[b]

[a]Ledbetter and Moment (Ref. 38).
[b]Wong *et al.* (Ref. 39).

generalization of the Vanderbilt ultrasoft pseudopotential and the linear augmented plane-wave[35] methods, i.e., the projector augmented wave technique. Within the PAW method, the all-electron wave functions are related to the pseudowave functions via a linear transformation.

We perform scalar-relativistic spin-polarized PAW calculations for Pu using the VASP code.[36] The calculations treat 16 valence electrons, including the semicore 6*s* and 6*p* states with a plane-wave cutoff of 23.4 Ry. As in the case of the FPLMTO, the SQS model is used for the disordered magnetic-moment configuration. Here, as opposed to in our previous work,[11] no lattice relaxations were allowed in the PAW. We calculate the PAW elastic constants and ZB phonons within the SQS8 and SQS16 models, respectively. The BZ is sampled with the same grid of *k* points for all the spin configurations, equivalent to a $12\times12\times12$ fcc Monkhorst-Pack grid.[37]

Even though the three presented numerical techniques are all founded on the same fundamental framework, the density-functional theory, they have distinct differences that give them certain advantages and disadvantages. First, the FPLMTO and VASP employ no approximations to the electron potential and charge density and are therefore somewhat more reliable for very open structures and/or small distortions. The FPLMTO includes spin-orbit and orbital polarization interactions and is therefore the most accurate method. PAW, however, is at least an order of magnitude faster than FPLMTO and can more easily be used to calculate forces due to the plane-wave basis set. Both these methods require the use of supercells to study disorder. The EMTO method, on the other hand, is well suited to study disordered systems within the CPA. The EMTO make some geometrical approximations in the construction of the electron potential, but these are controlled by the fact that it is optimized to best represent the full potential. The FPLMTO and EMTO do not assume any pseudopotential but calculate energy contributions from all electrons.

III. RESULTS AND DISCUSSION

The results are shown in Table I. Notice first that the calculations assuming a disordered magnetic state (*D*) predict very similar equilibrium volumes, 25.5 Å^3 (EMTO), 24.9 Å^3 (FPLMTO), and 23.9 Å^3 (PAW). Also the bulk moduli are in close agreement with each other 38, 41, and 46 GPa. In spite of their numerical differences, the methods predict very similar bonding properties which suggests that these DFT results are robust. Also the ferromagnetic (FM) FPLMTO treatment of δ-Pu appears to be reasonable with respect to equilibrium volume and bulk modulus. For comparison we also show results from a nonmagnetic (NM) calculations, i.e., no spin/orbital polarization and spin-orbit coupling, using the FPLMTO method. It is very obvious that neglecting magnetic effects predicts a serious overbinding with a too small equilibrium volume (29%) and too large bulk modulus (550%) as a result. Also, a negative C' suggests a mechanical instability of δ-Pu for this restricted calculation, which is clearly not suitable for δ-Pu.

Next, we discuss the calculated elastic constants, shown in Table I. These are considerably more sensitive to details of the calculations and this becomes clear when comparing the theoretical results. The tetragonal shear constant C' provides information regarding the stability of the cubic phase with respect to a tetragonal distortion. It is expected to be small because the δ' phase, which is a tetragonal phase, is stabilized when the δ phase is heated only about 100 K. The calculations of C', assuming a magnetic state, are all small ranging from 8.1 GPa to 18 GPa. The shear constant C_{44} is predicted to be considerably larger, ranging from 30 GPa to 81 GPa. The FM FPLMTO calculations predict a somewhat smaller value, 27 GPa. Overall, the elastic constants are consistently overestimated in the calculations compared to experiments, although the large and anomalous anisotropy ratio is relatively well reproduced assuming a disordered magnetic state: it is equal to 10 (EMTO), 2.7 (FPLMTO), and 3.0 (PAW), whereas ultrasonic[38] and x-ray[39] measurements indicate C_{44}/C' to be equal to 7.1 and 6.3, respectively. For uranium metal, calculated elastic constants[40,41] are also larger than experiment and part of the explanation in this case is the substantial temperature dependence of these constants. The present calculations refer to zero temperature whereas the measurements were recorded at room temperature. To our knowledge, no experiments of elastic constants for single-crystal δ-Pu at lower temperatures exist. For polycrystal δ-Pu elasticity was recently measured as a function of temperature near the room temperature.[42] These show a linear temperature dependence and, when extrapolated from room to zero temperature, they suggest an increase of the order of 20%. Taking this into

account, the FPLMO and PAW calculation of C' and the EMTO calculation of C_{44} are in greater discrepancy with experiment than what is typically found for elastic-constant calculations for metals in general (up to 20% error is expected). Incidentally, the present EMTO results are in a good agreement with those of LDA+U, where a strong localization of the $5f$ electrons is assumed, by Bouchet *et al.*[43] ($C'=12$ GPa and $C_{44}=75$ GPa).

The ZB phonons are calculated using the so-called frozen phonon method. This method require the study of supercells, where the total-energy response to the movement of an atom corresponding to the phonon mode, is calculated. This procedure is less suitable for our treatment of the disordered magnetic state in the FPLMTO (and PAW) methods because of the already large (eight atoms/cell) computation and for this reason we do not attempt this calculation using the FPLMTO. Notice in Table I that all calculations reproduce the correct numerical order of the ZB phonons, with the agreement between experiment and FPLMTO/PAW being rather good. The L_T phonon for the PAW treatment is too large, however. The EMTO method overestimates the ZB phonons consistently. Possible reasons for the discrepancy between theory and experiment may be that the measurements were made at room temperature on alloy stabilized δ-Pu, whereas theory deals with pure δ-Pu at zero temperature.

IV. SUMMARY

Disordered magnetism in conjunction with traditional density-functional formalism is a tool for describing elastic properties of paramagnetic δ-Pu. Because the present approach is fundamentally founded on density-functional theory, the results are robust, although rather sensitive to numerical approximations and implementations. The DFT-CPA-DLM technique is particularly useful because there is no need to study large supercells. In addition, this approach is well suited to study δ-Pu based alloys.

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[1] S. S. Hecker, D. R. Harbur, and T. G. Zocco, Prog. Mater. Sci. **49**, 429 (2004).
[2] P. Söderlind, J. M. Wills, B. Johansson, and O. Eriksson, Phys. Rev. B **55**, 1997 (1997).
[3] O. Eriksson, J. D. Becker, A. V. Balatsky, and J. M. Wills, J. Alloys Compd. **287**, 1 (1999).
[4] A. J. Arko, J. J. Joyce, L. Morales, J. Wills, J. Lashley, F. Wastin, and J. Rebizant, Phys. Rev. B **62**, 1773 (2000).
[5] S. Y. Savrasov, G. Kotliar, and E. Abrahams, Nature (London) **410**, 793 (2001).
[6] X. Dai, S. Y. Savrasov, G. Kotliar, A. Migliori, H. Ledbetter, and E. Abrahams, Science **300**, 953 (2003).
[7] P. Söderlind, Adv. Phys. **47**, 959 (1998).
[8] A. V. Postnikov and V. P. Antropov, Comput. Mater. Sci. **17**, 438 (2000).
[9] Y. Wang and Y. Sun, J. Phys.: Condens. Matter **12**, L31 (2000).
[10] P. Söderlind, Europhys. Lett. **55**, 525 (2001).
[11] P. Söderlind, A. Landa, and B. Sadigh, Phys. Rev. B **66**, 205109 (2002).
[12] A. Landa, P. Söderlind, and A. Ruban, J. Phys.: Condens. Matter **15**, L371 (2003).
[13] M. Dormeval, Ph.D. Thesis, Universite de Bourgogne, Dijon, France, 2001.
[14] P. Söderlind and B. Sadigh, Phys. Rev. Lett. **92**, 185701 (2004).
[15] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
[16] O. K. Andersen, O. Jepsen, and G. Krier, in *Methods of Electronic Structure Calculations*, edited by V. Kumar, O. K. Andersen, and A. Mookerjee (World Scientific, Singapore, 1994), pp. 6–124.
[17] O. K. Andersen, C. Arcangeli, R. W. Tank, T. Saha-Dasgupta, G. Krier, O. Jepsen, and I. Dasgupta, in *Tight-binding Approach to Computational Materials Science*, edited by P. E. A. Turchi, A. Gonis, and L. Colombo, M. R. S. Sympeosia Proceeding No. 491 (Materials Research Society, Warrendale, 1998), pp. 3–34.
[18] L. Vitos, H. L. Skriver, B. Johansson, and J. Kollar, Comput. Mater. Sci. **18**, 24 (2000).
[19] L. Vitos, Phys. Rev. B **64**, 014107 (2001).
[20] J. Kollar, L. Vitos, and H. L. Skriver, in *Electronic Structure and Physical Properties of Solids: The Uses of the LMTO Method*, edited by H. Dreysse, Lecture Notes in Physics Vol. 535 (Springer, Berlin, 2000), pp. 85–113.
[21] L. Vitos, I. A. Abrikosov, and B. Johansson, Phys. Rev. Lett. **87**, 156401 (2001).
[22] A. I. Landa, C.-C. Chang, P. N. Kumta, L. Vitos, and I. A. Abrikosov, Solid State Ionics **149**, 209 (2002).
[23] L. Vitos, P. A. Korzhavyi, and B. Johansson, Phys. Rev. Lett. **88**, 155501 (2002).
[24] A. Landa and P. Söderlind, J. Alloys Compd. **354**, 99 (2003).
[25] A. Landa and P. Söderlind, J. Alloys Compd. **376**, 62 (2004).
[26] B. L. Györffy, A. J. Pindor, G. M. Stocks, J. Staunton, and H. Winter, J. Phys. F: Met. Phys. **15**, 1337 (1985).
[27] D. J. Chadi and M. L. Cohen, Phys. Rev. B **8**, 5747 (1973); S. Froyen, *ibid.* **39**, 3168 (1989).
[28] F. D. Murnaghan, Proc. Natl. Acad. Sci. U.S.A. **30**, 244 (1944).
[29] M. J. Mehl, B. M. Klein, and D. A. Papaconstantopoulos, *Intermetallic Compounds: Principles and Practice: Principles*, edited by J. H. Westbrook and R. L. Fleischer (Wiley, London, 1995), Vol. 1, Chap. 9, pp. 195–210.
[30] P. Söderlind, J. Moriarty, and J. M. Wills, Phys. Rev. B **53**,

14 063 (1996).
[31] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, Phys. Rev. Lett. **65**, 353 (1990).
[32] D. R. Hamann, M. Schlüter, and C. Chiang, Phys. Rev. Lett. **43**, 1494 (1979).
[33] D. Vanderbilt, Phys. Rev. B **41**, 7892 (1990).
[34] P. E. Blöchl, Phys. Rev. B **50**, 17 953 (1994).
[35] D. J. Singh, *Pseudopotentials, and the LAPW Method* (Kluwer, Boston, 1994).
[36] G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993); G. Kresse and J. Furthmüller, *ibid.* **54**, 11 169 (1996); G. Kresse and D. Joubert, *ibid.* **59**, 1758 (1999).
[37] H. J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976).
[38] H. M. Ledbetter and R. L. Moment, Acta Metall. **24**, 891 (1976).
[39] J. Wong, M. Krisch, D. L. Farber, F. Occelli, A. J. Schwartz, T.-C. Chiang, M. Wall, C. Boro, and R. Xu, Science **301**, 1078 (2003).
[40] P. Söderlind, Phys. Rev. B **66**, 085113 (2002).
[41] A. L. Kutepov, LLNL Report No. UCRL-TR-200698, 2003 (unpublished).
[42] A. Migliori, D. A. Miller, J. C. Lashley, F. Freibert, J. B. Betts, and M. Ramos, in *Plutonium Futures—The Science*, edited by G. D. Jarvinen (AIP, Melville, NY, 2003), p. 73.
[43] J. Bouchet, B. Siberchicot, F. Jollet, and A. Pasturel, J. Phys.: Condens. Matter **12**, 1723 (2000).