Ab initio determination of the nuclear quadrupole moments of ^{114}In, ^{115}In, and ^{117}In

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We present here *ab initio* determinations of the nuclear-quadrupole moment Q of hyperfine-probe-nuclear states of three different In isotopes: the 5^+ 192 keV excited state of ^{114}In (probe for nuclear quadrupole alignment spectroscopy), the $9/2^+$ ground state of ^{115}In (nuclear magnetic and nuclear quadrupole resonance probe), and the $3/2^+$ 659 keV excited state of ^{117}In (perturbed angular correlations probe). These nuclear-quadrupole moments were determined by comparing experimental nuclear-quadrupole frequencies to the electric field gradient tensor calculated with high accuracy at In sites in metallic indium within the density functional theory. These *ab initio* calculations were performed with the full-potential linearized augmented plane wave method. The results obtained for the quadrupole moments of ^{114}In [$Q(^{114}\text{In}) = -0.14(1)\ b$] are in clear discrepancy with those reported in the literature [$Q(^{114}\text{In}) = +0.16(6)\ b$ and $+0.739(12)\ b$]. For ^{115}In and ^{117}In our results are in excellent agreement with the literature and in the last case $Q(^{117}\text{In})$ is determined with more precision. In the case of $Q(^{117}\text{In})$, its sign cannot be determined because standard γ-γ perturbed angular correlations experiments are not sensitive to the sign of the nuclear-quadrupole frequency.

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I. INTRODUCTION

Hyperfine interaction techniques, widely applied to the study of condensed matter physics, such as Mössbauer spectroscopy, nuclear magnetic and nuclear quadrupole resonance (NMR and NQR) or perturbed angular correlations (PAC), among others,[1–3] are based on the observation of the coupling between nuclear moments and extra-nuclear fields. These techniques are often used as a powerful tool to characterize precise atomic sites in a given sample and to obtain information about local symmetry, coordination, and valence of defect or native centers in solids, among other electronic, structural, and magnetic properties on a nanoscopic scale.[4] The electric-nuclear-quadrupole interaction, in particular, can give information on the electronic charge density $[\rho(r)]$ in a probe-host system. In such measurements the relevant information is contained in the electric field gradient (EFG) tensor acting at the probe nucleus, since the EFG tensor is directly related to the anisotropy of the electronic density in the close vicinity of the probe-nucleus.[5] Experimentally accessible, however, is only the product of the EFG and the nuclear-quadrupole moment Q, proportional to the so-called quadrupole coupling constant ν_Q.

All the information that ν_Q can provide about the system under study could be obtained by confrontation with an accurate prediction of the EFG, such as those obtained with *ab initio* electronic-structure calculations. Of course, accurate values of the nuclear-quadrupole moments Q are essential for a correct comparison between the experimentally "determined" EFG and its theoretical prediction. For this reason, the knowledge of reliable Q values is of great importance in atomic, molecular, and condensed matter physics, besides the direct interest in nuclear physics, where the determination of Q values can be used to check nuclear models. However, for many important probe nuclei, the Q values are not known or are known with limited accuracy and/or limited precision and their determination is still an open field of research. A compilation of nuclear-quadrupole moments can be found in the tables of Kauffman and Vianden,[2] Vianden,[6] Raghavan,[7] Pyykkö,[8] and Stone.[9]

Ideally, nuclear physics calculations, although theoretical, should provide direct values of the quadrupole moments. In recent years decisive progress has been achieved in the field of nuclear shell models, but state of the art shell-model calculations can only handle medium mass nuclei ($A = 50-60$).[10] For example, to our knowledge, no reliable nuclear model predictions of quadrupole moments of In isotopes have been reported in the literature. Other methods widely used to determine Q values are based on optical and atomic beam spectroscopies. To extract the Q values from the experimental hyperfine-structure constants, theoretical calculations of atomic wave functions are necessary and several assumptions are usually done (see, for example, Refs. 11 and 12). Another competitive method used up to two decades ago was based on the observation of the hyperfine structure of mesons.[13] The current best approach to determine Q (as it was pointed out in Ref. 14) is to use information of both experimental quadrupole coupling constants and reliable theoretical EFG calculations for the same probe-host system. The accuracy in these calculations was very difficult to obtain, because the EFG tensor strongly depends on the electronic density details in the subnanoscopic neighborhood of the probe nucleus. This electronic density can be described by the occupation of orbitals with different symmetry around the nucleus. Small differences in the order of 0.01 electrons in the occupation of a given orbital led to quite different EFG results. Thus, the theoretical method employed must be able to describe accurately the wave functions in the immediate vicinity of the nucleus where the EFG is calculated. For this reason, pseudopotential methods are not well suited for EFG calculations. So, first-principles cluster methods (with a sufficiently large cluster size to ensure the accurate description

of the total charge density in the vicinity of the nucleus) or band-structure methods are the correct way to calculate the EFG tensor.

For a long time the EFG has been calculated using the simple point-charge model (PCM). Since such calculations do not account for any onsite polarization, atomic Sternheimer antishielding factors are shown to describe core polarization. In the framework of the PCM, charge transfer effects are only crudely estimated, and covalence is completely neglected. In 1985, Blaha, Schwarz, and Herzig[15] showed that the density functional theory (DFT) based linearized augmented plane wave band structure method[16] (LAPW) was able to predict with high accuracy the EFG in simple solids from first principles. In the last decade, increasing computer power and progress in methodological development enabled calculations in more complex systems, for example ionic insulators like Li_3N,[15] hcp metals,[17] semiconductor oxides like Cu_2O (Ref. 18) or TiO_2,[19] high T_c superconductors,[20] or to model surfaces[21] or doped systems.[22,23] Moreover, this method proved to be accurate enough to determine with high accuracy nuclear-quadrupole moments by comparison of EFG calculations with the experimentally measured ν_Q values.[24–26] A similar approach, but using *ab initio* atomic calculations, is used in the works of Bieroń *et al.*[27] and Martínez-Pinedo *et al.*[10] It is important to mention here that Martínez-Pinedo *et al.* performed determinations of the nuclear-quadrupole moment of excited states of ^{54}Fe and ^{57}Fe using state of the art nuclear calculations and also DFT atomic models combined with Mössbauer experimental results. Both approaches yielded very similar results.[10]

In this work we present *ab initio* determinations of the nuclear-quadrupole moments of three nuclear states of In isotopes: the 5^+ 192 keV excited state of ^{114}In, the $9/2^+$ ground state of ^{115}In, and the $3/2^+$ 659 keV excited state of ^{117}In. All these nuclear states are used as nuclear probes in nuclear-quadrupole alignment (NQA) spectroscopy (^{114}In), NMR and NQR (^{115}In), and PAC experiments (^{117}In). These determinations were obtained comparing experimentally determined nuclear-quadrupole frequencies to the EFG calculated at In sites in metallic indium using the full-potential LAPW (FLAPW) method. As we will show, the obtained results are in clear discrepancy with those reported in the literature in the case of $Q(^{114}\text{In})$, and $Q(^{117}\text{In})$ is obtained with better precision. In the last isotope, the sign of Q cannot be determined because standard γ-γ perturbed angular correlations experiments are not sensitive to the sign of ν_Q. In the case of ^{115}In our Q values are in excellent agreement with those reported recently in the literature. We will also show that the use of the accepted negative ν_Q value for ^{115}In in metallic indium has produced a wrong determination of the accepted $Q(^{114}\text{In})$ value.

II. METHOD AND COMPUTATIONAL ASPECTS

The EFG tensor is a traceless symmetric tensor of rank two, defined as the second derivative (with respect to the spatial coordinates) of the Coulomb potential at the position of the nucleus. The Coulomb potential can be determined from the total charge density in the crystal by solving Poisson's equation. In this scheme, the EFG can be determined straightforwardly once the total charge distribution has been calculated. After diagonalization, the EFG tensor can be described by its major principal component, V_{33}, and the asymmetry parameter $\eta=(V_{11}-V_{22})/V_{33}$ (with the convention $|V_{11}|<|V_{22}|<|V_{33}|$). In the three cases that we will study here, the experimental quadrupole coupling constant ν_Q is related to V_{33} by:

$$\nu_Q = \frac{eQ}{h} V_{33}. \tag{1}$$

For the calculations presented in this paper we employed the WIEN97.10 implementation[28] of the FLAPW method in a scalar relativistic version without spin-orbit coupling. In this method, no shape approximation on either the potential or the electronic charge density is made, thus being specially suited for EFG calculations. A description of the EFG calculation within the FLAPW method has been extensively described in the literature (see, e.g., Ref. 29). For methodological purposes the unit cell is divided into nonoverlapping muffin-tin (MT) spheres with radius R_i and an interstitial region (IR). In the IR the wave functions are expanded into plane waves, while inside the MT spheres these plane waves are augmented by an atomiclike spherical harmonics expansion. The MT spheres radius used for the In atoms was 1.3 Å. An advantage of plane-wave-based methods is that the convergence of their basis set can be tested easily by including additional plane waves in the calculations. This was done for several cases here and well-converged solutions were found when the parameter RK_{MAX} (which controls the size of the basis set in these calculations) was equal to 9 (R is the smallest MT radius and K_{MAX} the largest wave number of the basis set). This value gives a well converged basis set consisting of 150 LAPW functions. In addition to the usual LAPW basis set, we also add local orbitals (LO) to include In-4d orbitals. Integration in reciprocal space was performed using the tetrahedron method taking 30 000 k points in the full Brillouin zone (BZ), which are reduced to 2176 k points in the irreducible wedge of the BZ (IWBZ). The correctness of the choice of these parameters was checked by performing calculations for other R_i, k-point sampling, and RK_{MAX} values. Finally, exchange and correlation effects were treated within DFT using either the local-density approximation (LDA)[30] or the generalized gradient approximation (GGA).[31]

III. RESULTS FOR THE EFG TENSOR AND DETERMINATION OF THE NUCLEAR-QUADRUPOLE MOMENTS

Metallic indium crystallizes in a distorted cubic close packing. The unit cell is tetragonal, $a=b=3.221$ Å, $c=4.933$ Å at 4.2 K ($a=b=3.253$ Å, $c=4.947$ Å at 300 K),[32] with two atoms in the body-centered positions $(0;0;0)$ and $(1/2;1/2;1/2)$. In this metal, due to the mentioned distortion, the twelve equidistant neighbors of the cubic close packing fall into one group of four In atoms at a distance of 3.24 Å and a group of eight not so near, at 3.37 Å. This is a

very simple unit cell and the low number of atoms enabled a convergence study with high precision.

Initially, we calculated the equilibrium lattice parameters using FLAPW. To obtain the equilibrium lattice parameters we mapped the energy surface as a function of a and c in order to obtain the lattice parameters corresponding to the minimum energy of the system. This minimum corresponded to $a=3.178$ Å and $c=4.887$ Å (LDA). A similar result was found using the GGA approximation for the exchange and correlation potential. These results are in good agreement with the experimental determinations, showing that the FLAPW method describes correctly the structure of metallic Indium, giving support to our EFG calculations.

Now we can present our results for the EFG tensor. We obtained (for the experimental lattice parameters at 4.2 K and for the muffin-tin radius, k-point sampling, and R_{KMAX} values detailed in the previous section) $V_{33}=+2.45\times10^{21}$ V/m^2 (for LDA) and $V_{33}=+2.39\times10^{21}$ V/m^2 (GGA). In both cases, $\eta=0.00$, according to the symmetry of the structure, fixed in the calculations. The orientation of V_{33} results parallel to the c axis, while V_{22} is parallel to the a axis (of course, due to the EFG tensor symmetry, V_{11} points parallel to the equivalent b axis).

In order to evaluate the convergence of our results, relevant to estimate the precision of the V_{33} values obtained, we performed calculations for different muffin-tin radii, k-point sampling, and basis-set size. The muffin-tin radius was varied from 1.1 Å to 1.6 Å, while in the case of the k-point sampling we performed calculations increasing the sampling from 10 000 k points in the BZ (726 k points in the IWBZ) to 45 000 k points (3078 k points in the IWBZ). In order to check the convergence of the basis set we performed calculations from $R_{KMAX}=6$ (45 LAPW functions for $R_i=1.3$ Å) to $R_{KMAX}=10$ (200 LAPW functions for the same radius). The conclusion of all these calculations is that, for $R_i=1.3$ Å, 30 000 k points, and $R_{KMAX}=9$, the convergence error in the EFG tensor components is smaller than 0.05×10^{21} V/m^2. We will take this value as the convergence error in our calculation. The difference between the results obtained with the LDA and the GGA approximations for the exchange and correlation potential is similar to this convergence error.

Once we present the results for the EFG tensor, we can discuss our results for the nuclear-quadrupole moments of In isotopes. As we shall see, we find it more convenient to describe the obtained results not following the increasing number of nucleons of the isotopes.

A. The $9/2^+$ ground state of ^{115}In

The magnitude of ν_Q in metallic In has been accurately determined over a large temperature range using NQR spectroscopy. The sensitive state was the ground state of ^{115}In. The obtained result was $\nu_Q=45.24(1)$ MHz at 4.2 K.[32–34] The magnitude of ν_Q was also determined at 300 K using NMR. The obtained result was $\nu_Q=29.50$ MHz (reported without error).[35] Magnitude and sign of ν_Q were afterwards determined, using NMR, by Thatcher and Hewitt.[36] The reported result was $\nu_Q=-45.36$ MHz (reported without error). We have to mention here that the sign of ν_Q was not measured directly. The arguments that led the authors to conclude that ν_Q is negative is based on a systematic constructed using experimental data coming from various In alloys.[36] If we accept the plausible negative sign for ν_Q and we use our FLAPW results for the EFG, we obtain $Q(^{115}\text{In})=-0.76(2)\ b$ in the case of the LDA and $Q(^{115}\text{In})=-0.78(2)\ b$ in the case of the GGA.

The nuclear-quadruple moment of the ground state of ^{115}In was reported in 1952 by Koster,[12] based on the combination of atomic-beam measurements and hyperfine-structure atomic calculations. The author applied three different methods of calculation and therefore obtained three values of $Q(^{115}\text{In})$: +1.17 b, +0.759 b, and +0.834 b. This last value was obtained with the more complete method that involved the splitting of the fine structure and this value was accepted as the best one. This value did not include shielding corrections.[12] After applying Sternheimer corrections one obtained $Q(^{115}\text{In})=+0.861(45)\ b$.[37] It is important to mention that in these determinations of $Q(^{115}\text{In})$ different assumptions were employed. A very recent determination of the nuclear-quadrupole moment of the ground state of ^{115}In in indium halides was reported by van Stralen and Visscher combining experimental direct determinations of magnitude and sign of quadrupole coupling constants and EFG calculations performed with state of the art molecular calculations.[38] The reported $Q(^{115}\text{In})$value was +0.770(8) b. As can be seen, these results for the nuclear-quadrupole moment of the ground state of ^{115}In are in clear contradiction with our Q values mentioned above. Giving confidence to our accurate EFG calculations in metallic In and those performed in In halides and also to the experimental sign determination of ν_Q in In halides, we conclude that the assumed sign of ν_Q of ^{115}In in metallic indium performed by Thatcher and Hewitt[36] must be wrong. Thus, our recommended values are $Q(^{115}\text{In})=+0.76(2)\ b$ in the case of the LDA and $Q(^{115}\text{In})=+0.78(2)\ b$ in the case of the GGA.

The excellent agreement between our Q values and those coming from molecular In systems (see Table I) is of great importance because the $Q(^{115}\text{In})$ value was used by different authors to determine Q values of many other nuclear states of In isotopes, as reported in the latest compilation of Stone.[9] A direct NMR determination of the sign of ν_Q at ^{115}In in metallic Indium must be done in order to unambiguously check the validity of our Q values and those reported in the literature.

B. The 5^+ 192 keV excited state of ^{114}In

The nuclear-quadrupole interaction of ^{114}In in metallic indium was determined by Brewer and Kaindl[39] using the nuclear quadrupole alignment (NQA) technique. While the sign determination is lacking in most experimental techniques, NQA gives a direct and straightforward determination of the sign of the quadrupole coupling constant ν_Q. The obtained result (at 4.2 K) was $\nu_Q=-8.4(3)$ MHz. Since the nuclear-quadrupole moment of the 192 keV excited state was not determined when this experiment was performed, from the above frequency the authors obtained a value of $Q(^{114}\text{In})=+0.16(6)\ b$, assuming the EFG to be negative.[39]

TABLE I. Results previously reported in the literature (see text) and those obtained in this work for the nuclear-quadrupole moment Q of different In isotopes.

Isotope and state	Q (literature)	Q (this work)
^{115}In$-9/2^+$ ground state	+1.17 b (Ref. 12) +0.759 b (Ref. 12) +0.834 b (Ref. 12) +0.770(8) b (Ref. 38)	+0.76(2) b (LDA)/+0.78(2) b (GGA)
^{114}In-5^+ 192 keV excited	+0.16(6) b (Ref. 39) +0.739(12) b (Ref. 40)	−0.14(1) b (LDA)/−0.15(1) b (GGA)
^{117}In$-3/2^+$ 659 keV excited state	±0.64(4) b (Ref. 37) ±0.58(6) b (Ref. 41)	±0.58(1) b (LDA)/±0.60(1) b (GGA)

Unfortunately, the authors did not discuss the method of calculation or the value employed for the major principal component of the EFG tensor. But it is simple to deduce, from the value they obtained for $Q(^{114}\text{In})$, that the authors employed the reported value of ν_Q obtained in metallic indium with the probe ^{115}In (see Ref. 36) and the quadrupole moment of ^{115}In reported by Koster[12] to obtain V_{33}. This value ($V_{33}=-2.18\times10^{21}$ V/m^2) was then used to obtain $Q(^{114}\text{In})$. Another reported value for the nuclear-quadrupole moment of ^{114}In is +0.739(12).[40] This value was obtained by collinear fast-beam laser spectroscopy. In this determination, several assumptions, as Sternheimer corrections, have had to be included.

If we use our FLAPW results for the EFG tensor at In sites in metallic indium and the reported experimental values of ν_Q for ^{114}In, we can obtain a value of $Q(^{114}\text{In})=-0.14(1)\ b$ in the case of the LDA and $Q(^{114}\text{In})=-0.15(1)\ b$ in the case of the GGA, in clear contradiction with the previously reported values[39,40] (see Table I). Giving confidence to our *ab initio* calculations of V_{33} and the direct determination of the magnitude and sign of ν_Q for ^{114}In in metallic In, the disagreement can only be attributed to the ν_Q sign assignment done by Thatcher and Hewitt[36] for ^{115}In in metallic indium, assignment used by Brewer and Kaindl[39] in the determination of $Q(^{114}\text{In})$.

C. The $3/2^+$ 659 keV excited state of ^{117}In

^{117}Cd and ^{117m}Cd decay by β^+ processes to excited states of ^{117}In. One of these excited states of ^{117}In, the 659 keV excited state, can be used as sensitive state in γ-γ PAC experiments. Using this technique, the magnitude of ν_Q in metallic In has been determined at different temperatures. The result obtained by Raghavan and Raghavan at 4.2 K was $\nu_Q=32.1(5)$ MHz [$\nu_Q=21.74(22)$ MHz at 295 K].[37] $\eta=0.00$ was assumed during the fitting of the spectra according to the crystal In structure. In these experiments, the concentration of ^{117}Cd($\rightarrow^{117}$In) probes was 1% ($In_{0.99}Cd_{0.01}$). The sign of the EFG tensor was not determined because standard γ-γ perturbed angular correlations experiments are not sensitive to the sign of the nuclear-quadrupole frequency. Hence it will not be possible to determine the sign of $Q(^{117}\text{In})$ from this measurement.

As we said before, the usual problem in the determination of the quadrupole moments in the approach we are using in this work was the lack of reliable estimations of the EFG tensor although the quadrupole interaction frequency could be measured accurately. Raghavan and Raghavan[37] eliminated the need to know the EFG by the fact that NQR experimental results on ^{115}In in $In_{0.99}Cd_{0.01}$ were known at that time. In effect, Thatcher and Hewitt[36] have made NMR measurements in this compound at 4.2 K. They report $\nu_Q=43.2(1)$ MHz. Thus, the ratio $Q(^{117}\text{In})/Q(^{115}\text{In})$ was derived to be, in absolute value, 0.743(15). Using the value of the nuclear-quadrupole moment of the ground state of $Q(^{115}\text{In})$ reported in the literature[12] and after applying a Sternheimer correction of 3.2%, Raghavan and Raghavan obtained $Q(^{117}\text{In})=0.64(4)$ b.[37] A similar result was obtained by Haas and Shirley [$Q(^{117}\text{In})=0.58(6)\ b$].[41] We have to mention here that the determination of $Q(^{117}\text{In})$ performed by Raghavan and Raghavan is based on the nuclear-quadrupole moment of the ground state of ^{115}In reported at that time.

Using the experimental value of ν_Q at 4.2 K and our first-principles theoretical values for V_{33}, we found $Q(^{117}\text{In})=0.58(1)\ b$ (LDA), $Q(^{117}\text{In})=0.60(1)\ b$ (GGA), without the use of arbitrary corrections. These results are summarized in Table I. As can be seen, our Q values for ^{117}In are more precise than those obtained in Refs. 37 and 41 from the ratio $\nu_Q(^{117}\text{In})\times Q(^{115}\text{In})/\nu_Q(^{115}\text{In})$ using the reported $Q(^{115}\text{In})$ value of Ref. 12. If we use our $Q(^{115}\text{In})$ value in this ratio we obtain $Q(^{117}\text{In})=0.57(2)\ b$ in very good agreement with our *ab initio* result.

IV. CONCLUSIONS

In the present work we have presented very precise *ab initio* electronic-structure FLAPW calculations for the EFG tensor at In sites in metallic indium. The combination of experimental hyperfine interaction measurements with these accurate theoretical EFG calculations enables us to determine the nuclear-quadrupole moment Q of different nuclear

states of In isotopes, which can be used as sensitive states in different experimental techniques widely employed in condensed matter. These determinations are vital for the interpretation of experimental results in atomic, molecular, and solid-state physics since the knowledge of the Q value enables the EFG tensor to be extracted from the experimental measurement of ν_Q. These EFGs can then be used to validate the physical properties predicted by state of the art electronic-structure calculations in solids, atoms, and molecules. In addition Q values determined using nowadays simple calculations such as those presented here, can be used in nuclear physics to check the predictions of nuclear models.

Our results for $Q(^{115}\mathrm{In})$ are in excellent agreement with independent results coming from the combination of ν_Q values and EFG calculations in molecular In halides. This validation of the $Q(^{115}\mathrm{In})$ accepted value is of great importance because $Q(^{115}\mathrm{In})$ was used by different authors to determine Q values of many other nuclear states of In isotopes. From these results we can infer that the accepted ν_Q sign for $^{115}\mathrm{In}$ in metallic indium is wrong. A direct NMR determination of this sign must be done in order to unambiguously check the validity of our Q values and those reported in the literature. Our results for $Q(^{114}\mathrm{In})$ are in clear contradiction with those reported in the literature. This disagreement can only be attributed to the use of the wrong sign of ν_Q for $^{115}\mathrm{In}$ in metallic indium in the determination of $Q(^{114}\mathrm{In})$. The agreement between our Q value for $^{117}\mathrm{In}$ and the previously reported one seems to be rather good in magnitude, although our result is more precise.

We think that the results presented here should stimulate experimental determinations of the sign and magnitude of ν_Q in metals and simple systems, in particular $^{115}\mathrm{In}$ in metallic indium. In effect, many nuclear-quadrupole moments of different nuclear states of In isotopes, quoted in the latest nuclear-quadrupole-moment compilations, are based on the previously reported $Q(^{115}\mathrm{In})$ value, which are currently being used to check, e.g., *ab initio* theoretical calculations in condensed matter physics.

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