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Abstract
An *ab initio* approach to the magnetic properties of bulk hexagonal Gd is
developed that is based on the local spin-density approximation with the 4f
electrons treated as localized core electrons. The effective one-electron problem
is solved using the tight-binding linear muffin-tin orbital method in the atomic-
sphere approximation with the valence basis consisting of s-, p- and d-type
orbitals. The approach leads to a correct description of the ground-state
properties like the stability of the ferromagnetic structure, the magnetic moment
and the equilibrium lattice constant. Application of a real-space Green-function
formalism yields the exchange pair interactions between distant neighbours that
are inevitable for quantitative studies of magnetic excitations. The distance
dependence and anisotropy of the exchange pair interactions are presented
and the Curie temperature in the mean-field approximation is evaluated. The
obtained value of 334 K is in much better agreement with the experimental
value of 293 K than previous theoretical results. Depending on the atomic
volume we find an unusually large dependence of the Curie temperature on the
c/a ratio, which bears important consequences for the critical temperatures of
thick strained Gd films as grown on various substrates.

1. Introduction

The magnetic properties of bulk gadolinium in a hexagonal close-packed (hcp) structure
represent a serious test for *ab initio* theories based on the local spin-density approximation
(LSDA) [1] to the density-functional theory [2]. It was found that application of the LSDA
to this f-electron system predicts an incorrect magnetic ground-state structure, namely the

antiferromagnetic (AFM) stacking of the (0001) atomic layers, in contrast to the observed ferromagnetic (FM) state [3]. A number of schemes were suggested to overcome this failure of LSDA due to the highly localized nature of the valence 4f orbitals. The most systematic and successful approach explicitly includes the Coulomb parameter U for the 4f electrons (LSDA+U) [4–7] which stabilizes the FM order. Gradient corrections to the LSDA improve the situation when combined with the atomic-sphere approximation (ASA) [3, 8, 9] whereas their effect within a full-potential method is not strong enough to stabilize the FM structure [9, 10]. The simplest approach yielding the correct FM ground state is based on a treatment of the 4f states as part of the core [10, 11]. A recent detailed study by means of the full-potential augmented plane-wave (FLAPW) method revealed the origin of the AFM coupling in the LSDA: a large density of states at the Fermi level due to the minority 4f electrons [12]. The success of the various schemes described above can be thus explained by removing the minority 4f states from the neighbourhood of the Fermi energy while other features become less important in this respect.

The standard LSDA also fails in a quantitative treatment of the finite-temperature electronic properties of FM metals [13]. Selected aspects of the effect of finite temperatures on the electronic structure of Gd were recently addressed in terms of a many-body Hamiltonian model (Kondo-lattice model), the parameters of which were constructed from an *ab initio* band-structure calculation at zero temperature [14]. However, the resulting quantitative temperature dependence of the quasiparticle spectrum rests on a knowledge of the Curie temperature of hcp Gd. A parameter-free reproduction of the observed Curie temperature, $T_C = 293$ K [15], is thus another challenge for first-principles theories. The most sophisticated approach to the Curie temperature is based on the calculation of magnetic susceptibility in the paramagnetic state approximated by the so-called disordered local moment (DLM) state with local magnetic moments of a fixed magnitude but pointing in random directions [13]. This scheme was applied to the cubic 3d transition metals Fe and Ni [13, 16]. A simpler approach starts from the FM ground state and it maps the energy changes accompanying infinitesimal deviations of the local moment directions on to an effective classical Heisenberg Hamiltonian [17–19] from which the Curie temperatures, spin-wave stiffness constants and magnon dispersion laws can be derived. Both schemes were successful for Fe and Co but their applicability to Ni was problematic due to its small exchange splitting. For Gd however, a theory based on intraatomic exchange integrals was formulated within the LSDA [20] which provided values of the Curie temperature in a wide interval between 172 and 1002 K, depending on the further approximations employed [20]. An alternative estimation of the Curie temperature can be based on mapping the calculated total energies of different spin configurations on to a Heisenberg Hamiltonian. This approach has recently been applied to hcp Gd by taking into account only the FM and AFM magnetic orders [12]. Despite a narrower interval found for the resulting Curie temperatures (between 263 and 464 K), the reliability of this and similar schemes is usually limited due to a finite number of spin configurations (mostly collinear) used for the mapping.

The present paper aims at a more systematic *ab initio* approach to the magnetic properties of hexagonal Gd, namely a treatment based on the pairwise Heisenberg Hamiltonian with parameters derived from a self-consistent electronic structure of the FM ground state using the magnetic force theorem [17–19, 21]. The electronic structure is calculated within the LSDA but with the 4f orbitals included in the atomic-like core. We investigate the distance dependence and anisotropy of the exchange interactions and calculate the Curie temperature in a mean-field approximation (MFA). We find that the latter is in reasonable agreement with experiment, in full analogy with previous results for Fe and Co [19]. This fact confirms the applicability of the Heisenberg model to hcp Gd due to its large magnetic moments with magnitudes that are nearly insensitive to the magnetic order.

2. Formalism and numerical details

The self-consistent electronic structure calculations were performed using the all-electron scalar-relativistic tight-binding linear muffin-tin orbital (TB-LMTO) method in the ASA [22, 23]. The exchange-correlation potential was parameterized according to [24] and the Brillouin-zone (BZ) integrals were evaluated using 2030 k-points in the irreducible wedge of the hcp BZ. The valence basis comprised s-, p- and d-type orbitals, whereas the 4f orbitals were described as core orbitals. Since the latter lie close to the Fermi energy, a modified boundary condition to the single-site eigenvalue problem has to be supplied. It was formulated as $D_\ell(E) = -\ell - 1$, where $\ell = 3$ and $D_\ell(E)$ denotes the logarithmic derivative of the solution to the radial Schrödinger equation at the atomic-sphere boundary. This condition defines the centre of a pure (unhybridized) ℓ-band of the LMTO–ASA method [25]. The occupancy of the 4f level was fixed at the observed half-filled shell; the majority (minority) 4f level was fully occupied (empty).

The accuracy of the ASA for the self-consistent calculations was checked by the FLAPW method which enables us to also perform standard LSDA (with 4f orbitals in the valence basis) as well as LSDA + U calculations. Their results were reported in detail elsewhere [12].

The exchange interactions were investigated in a framework of an effective Heisenberg Hamiltonian

$$H_{\text{eff}} = -\sum_{RR'} J_{RR'} e_R \cdot e_{R'}, \tag{1}$$

where the subscript R labels the lattice sites, the vectors e_R are unit vectors pointing in the direction of the individual local moments and the pair exchange interactions $J_{RR'}$ satisfy $J_{RR'} = J_{R'R}$ and $J_{RR} = 0$. They can be calculated using the magnetic force theorem [17, 21] applied within the TB-LMTO–ASA method [19] as

$$J_{RR'} = -\frac{1}{8\pi i} \int_C \text{tr}_L \left[\Delta_R(z) g_{RR'}^\uparrow(z) \Delta_{R'}(z) g_{R'R}^\downarrow(z) \right] dz. \tag{2}$$

In (2), the symbol tr_L denotes the trace over the angular momentum index $L = (\ell m)$ and energy integration is performed in the complex energy plane along a closed contour C starting and ending at the Fermi energy (with the occupied part of the valence band lying inside C). The quantities $g_{RR'}^\sigma(z)$ (σ being a spin index, $\sigma = \uparrow, \downarrow$) denote site-off-diagonal blocks of the so-called auxiliary Green-function matrices with elements $g_{RL,R'L'}^\sigma(z)$ while $\Delta_R(z) = P_R^\uparrow(z) - P_R^\downarrow(z)$ are diagonal matrices related to the potential functions $P_{R\ell}^\sigma(z)$ of the TB-LMTO–ASA method [23]. The parameters $J_{RR'}$ determined by (2) do not contain contributions due to constraining fields necessary to keep the frozen non-collinear spin structure a stationary state of the Kohn–Sham equation. We believe that due to the large magnetic moment of Gd and its small sensitivity to different spin arrangements (see below), these contributions can be neglected.

In the case of an FM system with all lattice sites equivalent, the Curie temperature in the MFA for the classical Hamiltonian (1) is given by

$$k_B T_C^{\text{MFA}} = \tfrac{2}{3} J_0, \tag{3}$$

where k_B is the Boltzmann constant and

$$J_0 = \sum_R J_{0R} \tag{4}$$

is an on-site exchange parameter related to the energy change due to an infinitesimal rotation of a single local moment with respect to the bulk magnetization [17]. The lattice summation

Table 1. Ground-state properties of hcp Gd as calculated in a 4f core treatment and with an experimental value of the c/a ratio ($c/a = 1.597$) for different spin structures: equilibrium WS radius (relative to the experimental value $s = 3.762$ au), bulk modulus, local magnetic moment and the energy difference with respect to an FM ground state.

Technique	State	$\Delta s/s$ (%)	B (Mbar)	M (μ_B)	ΔE (mRyd/atom)
LMTO–ASA	FM	−1.3	0.46	7.67	0.0
	AFM	−1.5	0.45	7.45	2.92
	DLM	−1.5	0.45	7.44	3.12
FLAPW	FM	−1.4	0.50	7.41	0.0
	AFM	−1.7	0.49	7.32	4.12
Experiment	FM	0.0	0.40	7.63	0.0

in (4) can be done exactly by employing a sum rule [17] to give

$$J_0 = \frac{1}{8\pi i} \int_C \text{tr}_L \left\{ \Delta_R(z) \left[g_{RR}^{\uparrow}(z) - g_{RR}^{\downarrow}(z) \right] + \Delta_R(z) g_{RR}^{\uparrow}(z) \Delta_R(z) g_{RR}^{\downarrow}(z) \right\} dz, \qquad (5)$$

which involves only the site-diagonal blocks of the Green-function matrices.

Reliable evaluation of the exchange interactions $J_{RR'}$ for interatomic distances $d = |R - R'|$ up to $d_{max} = 7a$, where a is the hcp lattice constant, requires typically a few millions of k-points in the full BZ averages defining the site-off-diagonal blocks $g_{RR'}^{\sigma}(z)$ [23]. The convergence property of the real-space sum in (4) was checked by the sum rule (5), sufficient accuracy of which is achieved by calculating the site-diagonal blocks $g_{RR}^{\sigma}(z)$ using a few thousands of k-points in the irreducible wedge of the BZ.

3. Results

3.1. Ground-state properties

Employing the above-described 4f core scheme in the TB-LMTO–ASA method, we performed calculations of total energies for hcp Gd as a function of the Wigner–Seitz (WS) radius s with the c/a ratio fixed at its experimental value, $c/a = 1.597$ (the measured lattice parameters are $a = 3.629$ Å and $c = 5.796$ Å [26]). The calculations assumed three different spin arrangements: besides the FM and AFM structures, the DLM state was considered and its electronic structure was calculated in the coherent-potential approximation [23]. The results are summarized in figure 1 and in table 1. The stabilization of the FM state is obvious: the energy separation of the AFM and DLM states with respect to the FM ground state amounts to 3 mRyd/atom. Note that the latter quantity is of a correct order of magnitude as compared to the experimental Curie temperature (293 K, 1 mRyd ≡ 158 K).

The theoretical equilibrium value of the WS radius s is not too sensitive to the spin structure (table 1) and its value for the FM state ($s = 3.712$ au) is merely 1.3% smaller than the experimental value ($s = 3.762$ au) while the calculated bulk modulus ($B = 0.46$ Mbar) is about 15% bigger than the measured one ($B = 0.40$ Mbar [27]). These values fall within the usual error bar of the standard LSDA and they agree with full-potential results of [10, 12].

The calculated local magnetic moment in the FM ground state is $M = 7.67 \, \mu_B$ (table 1) which compares very well with the experimental value of $M = 7.63 \, \mu_B$ [15]. The FLAPW method yields a slightly smaller value of $M = 7.41 \, \mu_B$ which can be ascribed to the different sphere radii used in the two techniques: the muffin-tin and WS spheres in the FLAPW and TB-LMTO methods, respectively. Inclusion of the interstitial contribution in the FLAPW method yields a total moment of $M = 7.80 \, \mu_B$/atom. Similar quantitative agreement with experiment
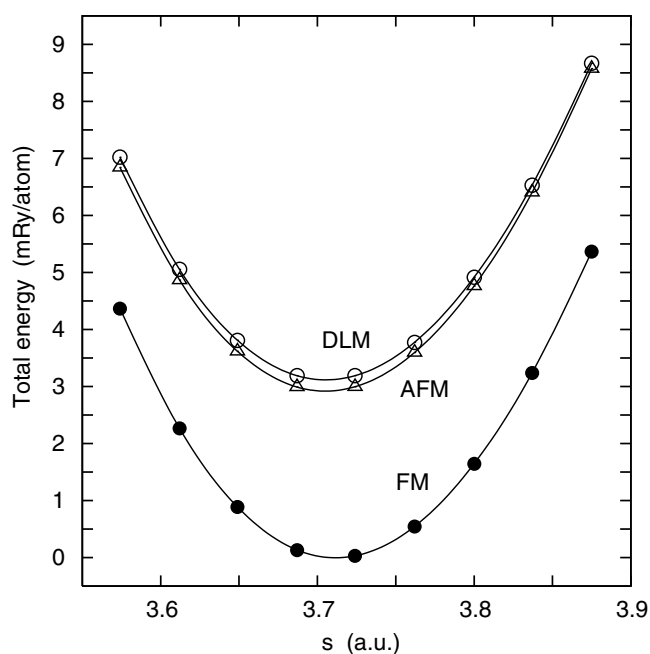
Figure 1. Total energy as a function of the WS radius *s* for hcp Gd with an experimental *c*/*a* ratio (*c*/*a* = 1.597) in the 4f core model for different magnetic states: FM (full circles), AFM (triangles) and DLM state (empty circles).

for the magnetization was obtained in previous 4f core calculations [10, 11]. Sensitivity of the local moments to the spin structure (table 1) reflects corresponding changes in spd bands, however, the relative changes of the moment magnitude (3%) are negligible due to the large and constant 4f contribution.

The spin-polarized densities of states (DOS) for the FM state with the theoretical equilibrium WS radius (*s* = 3.712 au) are shown in figure 2 together with positions of the 4f eigenvalues. The DOS shapes and the location of both 4f levels agree reasonably with those obtained by the FLAPW method [12]. Note especially the small difference between the minority 4f eigenvalue and the Fermi energy; an inclusion of f-type orbitals into the valence basis set would immediately lead to a pronounced enhancement of the minority DOS at the Fermi level which in turn stabilizes the AFM structure.

A detailed inspection of the results reveals an internal inconsistency of the 4f core treatment: for WS radii *s* larger than the experimental one, the minority 4f eigenvalue becomes lower than the Fermi energy, which violates the Kohn–Sham rule to occupy the lowest one-electron states in constructing the charge and spin density. Since this failure is documented in the literature [28], we have not tried to improve the situation, e.g., by modifications of the single-site boundary condition. As a reasonable reproduction of the most important ground-state properties was achieved within the present as well as previous 4f core treatments [10–12], the resulting self-consistent electronic structure was used in the following study of exchange interactions.
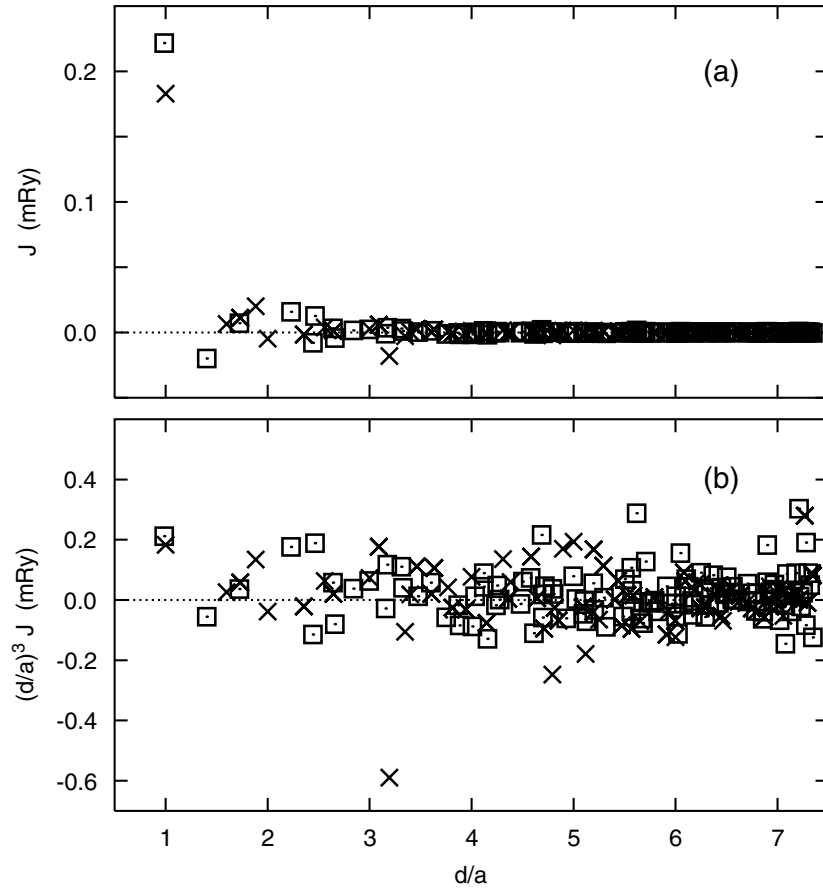
3.2. Exchange interactions

The exchange interactions were calculated from the self-consistent electronic structure of the FM state for a set of lattice constants *s* and *c*/*a* in a neighbourhood of their experimental values
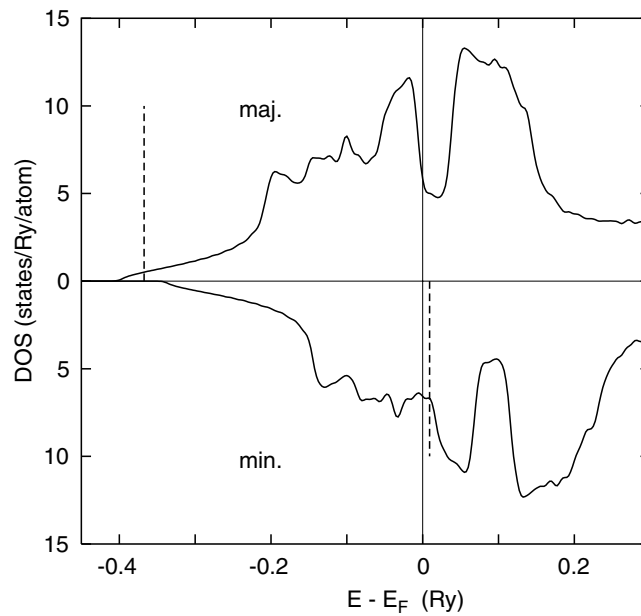
Figure 2. Spin-polarized densities of spd states for hcp Gd in an FM state with a theoretical equilibrium WS radius ($s = 3.712$ au). The zero on energy scale coincides with the Fermi energy. The dashed vertical lines mark positions of atomic-like 4f levels.

($s = 3.762$ au, $c/a = 1.597$). A typical dependence of the resulting pair interactions $J_{RR'}$ on the interatomic distance $d = |\boldsymbol{R} - \boldsymbol{R}'|$ is shown in figure 3(a) for the experimental value of c/a and the theoretical equilibrium value of s ($s = 3.712$ au). The first nearest neighbouring Js are positive and dominate clearly over the interactions of more distant pairs which oscillate and tend rapidly to zero with increasing distance d. The same qualitative features were found for the transition-metal ferromagnets bcc Fe, fcc Co and fcc Ni [19]. An analysis of (2) in the limit of large distances d reveals a Ruderman–Kittel–Kasuya–Yoshida (RKKY) asymptotic behaviour [19]. This is illustrated in figure 3(b) which proves undamped oscillations of the quantity $|\boldsymbol{R} - \boldsymbol{R}'|^3 J_{RR'}$. This behaviour agrees qualitatively with an experimentally found decrease of $J_{RR'}$ as $|\boldsymbol{R} - \boldsymbol{R}'|^{-3}$ reported for the rare-earth metals Gd, Tb and Dy [29]. The negative exchange interaction between the second nearest neighbours (figure 3) is also in qualitative agreement with experiment [29]. The latter fact refers to a pre-asymptotic region from a point of view of the RKKY theory.

Let us focus on the dominating first nearest-neighbour interactions. As can be seen in figure 3(a), they exhibit a non-negligible anisotropy: the exchange constant in the close-packed (0001) planes, $J_\parallel$, is about 20% smaller than that between these planes, $J_\perp$. Note that a 10% relative deviation was inferred in [12] from the total energy calculations for varying c/a ratio performed in [8] whereas an analysis of spin-wave dispersion relations measured at 77 K leads to an opposite relation [29]: $J_\parallel$ is about 20% bigger than $J_\perp$. The full calculated dependence of both exchange constants on the lattice parameters is presented in figure 4. While their dependences on s (for a fixed c/a ratio) are non-monotonous and not fully understood at present, the dependences on c/a (for a fixed s) are relatively simple: the exchange interaction $J_\parallel$ ($J_\perp$) increases (decreases) with increasing c/a ratio (see figures 4(a), (b)). This 'natural' behaviour suggests that the anisotropy of $J_\parallel$ and $J_\perp$ is mainly due to the deviation of a particular

Figure 3. Exchange interactions $J_{RR'}$ for FM hcp Gd with a theoretical equilibrium WS radius ($s = 3.712$ au) and an experimental c/a ratio ($c/a = 1.597$) as a function of the interatomic distance $d = |\boldsymbol{R} - \boldsymbol{R}'|$, without (a) and with (b) a prefactor d^3. The crosses and squares correspond to sites $\boldsymbol{R}, \boldsymbol{R}'$ lying in even (AA) and odd (AB) close-packed (0001) planes, respectively.

c/a ratio from its ideal value $c/a = 1.633$. This idea is corroborated by calculations performed for the ideal c/a ratio with varying s. As shown in figure 5, the resulting difference between $J_{\parallel}$ and $J_{\perp}$ is quite small indeed, especially for WS radii that are not too small ($s > 3.7$ au).

3.3. Curie temperatures

The resulting exchange interactions yielded directly the Curie temperature in the MFA (3) where the parameter J_0 was calculated both according to (4) with the real-space sum taken over all lattice sites within a cut-off distance $d_{max} = 7a$, and according to (5). The two approaches did not differ by more than 1% and the values of T_C^{MFA} for varying s and c/a are shown in figure 6(a). For the experimental lattice constants ($s = 3.762$ au, $c/a = 1.597$), the resulting value amounts to $T_C^{MFA} = 334$ K which is about 14% above the experimental value ($T_C = 293$ K). The dependence of T_C^{MFA} on s is rather weak (see figure 6(a)) yielding, for example, for the theoretical equilibrium value of s ($s = 3.712$ au) an increase to $T_C^{MFA} = 341$ K. This degree of agreement between theory and experiment is surprisingly satisfactory especially
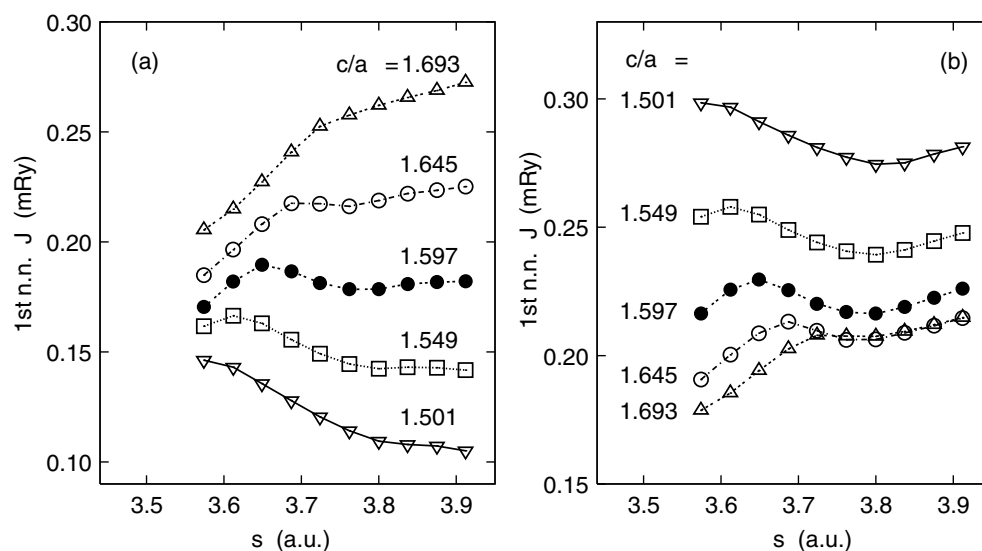
Figure 4. Exchange interactions between the first nearest neighbours of hcp Gd as functions of the WS radius s and the c/a ratio for neighbours located in one (0001) plane (a) and in two adjacent (0001) planes (b).
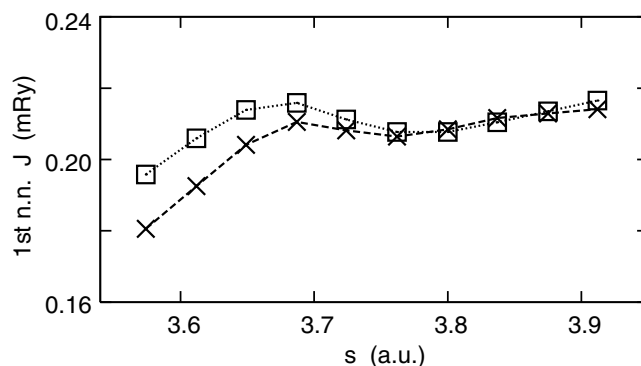

Figure 5. Exchange interactions between the first nearest neighbours of hcp Gd as functions of the WS radius s for the ideal c/a ratio ($c/a = 1.633$). The crosses and squares correspond to neighbours located in one (0001) plane and in two adjacent (0001) planes, respectively.

if one takes into account the well-known tendency of the MFA to overestimate the transition temperatures, in comparison to more accurate treatments. As was shown for Co and Ni in fcc structure [19], a random-phase approximation reduces the Curie temperature typically by 10–20% with respect to the MFA value. Assuming a similar reduction in the case of hcp Gd would shift the Curie temperature to between 270 and 300 K, i.e., even closer to experiment. Detailed calculations remain to be performed.

The dominating magnitudes of the first nearest-neighbour Js over the other atomic pairs represent an attractive feature which justifies various phenomenological spin Hamiltonians with nearest-neighbour interactions. However, an attempt to reproduce the T_C^{MFA} solely from the first nearest-neighbour Js included in the real-space sum (4) reveals the limited validity of such
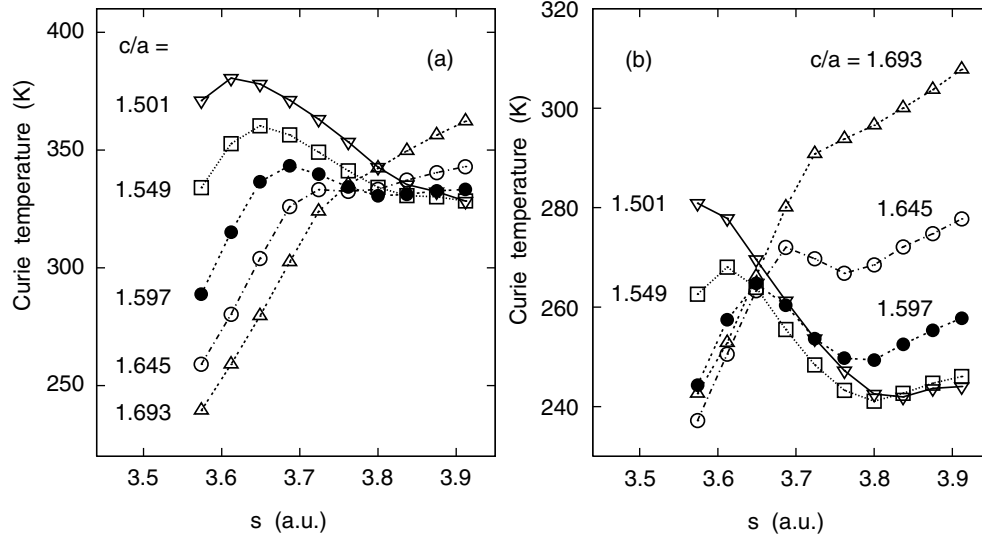
Figure 6. The Curie temperature of hcp Gd in the MFA as a function of the WS radius s and the c/a ratio with the summation in (4) carried out over all lattice sites (a) and restricted to the first nearest neighbours (b).
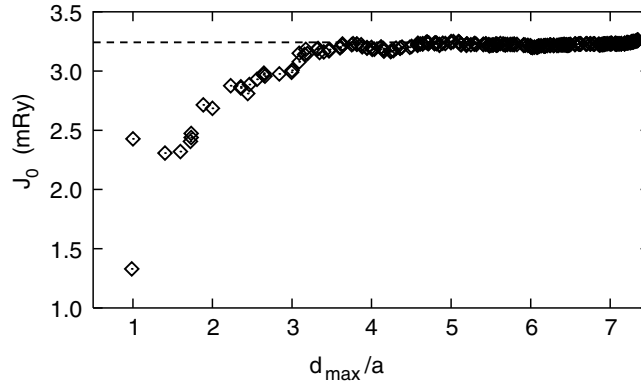

Figure 7. The on-site exchange parameter J_0 for the same lattice parameters as in figure 3 as a function of the cut-off distance d_{max} used in the lattice summation in (4). The dashed horizontal line denotes the exact value of J_0 from the sum rule (5).

approaches, as follows from comparison of figures 6(a) and (b). Neither the values of T_C^{MFA} nor their trends can be safely reproduced from the first nearest-neighbour interactions only.

This failure cannot be removed by including the second nearest neighbours; the corresponding exchange interaction is negative (cf figure 3) and the difference between the values in figures 6(a) and (b) would become even bigger. As shown in figure 7, quite a high number of neighbouring shells is necessary in order to get well-converged values of the on-site exchange parameter J_0 (4). The analysis performed proves the importance of the smaller interactions between distant atoms for a quantitative theory of itinerant magnetism.

The Curie temperatures can also be roughly estimated from the calculated energy differences between the AFM and FM states [12] or between the DLM and FM states according
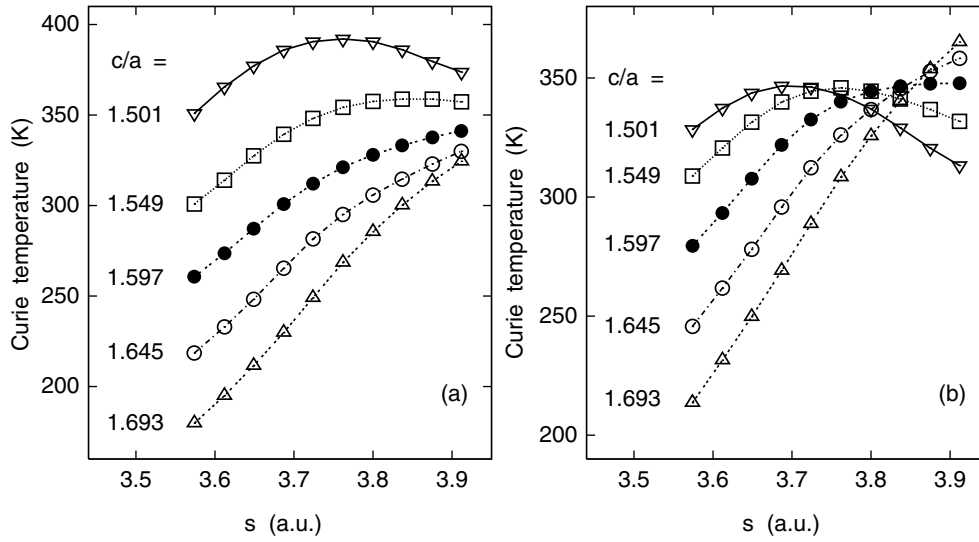
Figure 8. The Curie temperature of hcp Gd estimated from differences of total energies according to (6) as a function of the WS radius s and the c/a ratio from the AFM–FM difference (a) and from the DLM–FM difference (b).

to a simple formula

$$k_B T_C = \tfrac{2}{3}(E_{\text{AFM(DLM)}} - E_{\text{FM}}), \qquad (6)$$

where E_X is the total energy per atom in a magnetic state X, $X =$ FM, AFM, DLM. This approach can be justified on the basis of (3) if one identifies the parameter J_0 (4) with the DLM–FM energy difference per atom. In the case of the AFM–FM energy difference, one has to assume that the pair exchange interactions couple only the first nearest neighbours and that the anisotropy of the corresponding Js is negligible ($J_\parallel = J_\perp$) [12]. The Curie temperatures calculated according to (6) are presented in figure 8. A comparison of the values and the trends in figures 6 and 8 leads to a conclusion that the DLM–FM energy separation (figure 8(b)) provides a much better measure for the T_C^{MFA} (figure 6(a)) than the remaining two estimations based on neglecting the exchange interactions beyond the first nearest neighbours (figures 6(b), 8(a)).

The calculated values of T_C (figure 6(a)) exhibit quite a strong dependence on the c/a ratio, especially for small WS radii ($s \leqslant 3.7$ au). This feature can be related to recent measurements of T_C for strained epitaxial Gd(0001) films grown on various transition-metal substrates such as bcc W(110) [30, 31] and Nb(110) [32] and hcp Y(0001) [33]. As a rule, the Curie temperature of these films is smaller than those of bulk Gd. The thickness dependence of T_C is similar in all three cases studied but the measured values depend on the substrate as well. For example, the suppression of the Curie temperature for 30 Å Gd films amounts to $\Delta T_C \approx 7$, 20 and 50 K for the Y, Nb and W substrate, respectively, and the relation $\Delta T_C^Y < \Delta T_C^{\text{Nb}} < \Delta T_C^W$ holds in a broad interval of film thickness [33]. Since the lattice mismatch in the (0001) plane between the hcp lattices of Gd and Y is very small ($\approx 0.5\%$) [33], the measured ΔT_C reflects mainly the finite film thickness. In the case of W(110), the large lattice mismatch results in a sizeable compression of the Gd(0001) layers (4.4%) [30] which is partially compensated by an increase of the c/a ratio thus contributing to the large observed value of ΔT_C. The Nb(110) substrate is qualitatively similar to W(110) but with smaller ΔT_C due to the slightly bigger bcc lattice constant of Nb compared with W.

3.4. Properties of fcc Gd

We have also investigated properties of a hypothetical fcc Gd. The fcc and hcp lattices differ from the second nearest neighbours on and so a comparison of the exchange interactions and the Curie temperature can provide additional evidence for the structural sensitivity of the magnetic properties of bulk Gd. We found the equilibrium WS radius of fcc Gd to be $s = 3.693$ au, i.e., at an atomic volume only slightly smaller than that for hcp Gd with the ideal c/a ratio ($s = 3.712$ au). The local magnetic moment of fcc Gd, $M = 7.52\ \mu_B$, is close to that of hcp Gd ($M = 7.67\ \mu_B$). However, the first nearest neighbour exchange constant amounts in the fcc lattice to $J_1 = 0.123$ mRyd compared with the hcp value $J_1 \approx 0.21$ mRyd (for the ideal c/a ratio and neglecting the difference between the exchange constants $J_\parallel$ and $J_\perp$, cf figure 5). The calculated Curie temperature of fcc Gd is only $T_C^{\text{MFA}} = 92$ K which is substantially lower than the hcp value ($T_C^{\text{MFA}} = 333$ K). The big differences between the fcc and hcp values of J_1 and T_C^{MFA} represent an analogy with the strong dependence of the exchange interactions and the Curie temperature on the c/a ratio in hcp Gd.

4. Conclusions

We presented results of *ab initio* calculations for bulk hcp Gd focused on the exchange interactions in the FM ground state. This state was successfully described within the LSDA but with localized 4f orbitals treated as a part of the atomic core. The exchange interactions in the framework of an effective classical Heisenberg model were derived by applying the magnetic force theorem. They exhibit an RKKY asymptotic behaviour for large interatomic separations while the positive (FM) interactions between the first nearest neighbours dominate markedly over the other pair interactions. Calculations for varying lattice constants of the hcp structure reveal that the anisotropy in the first nearest-neighbour interactions is mainly due to the deviation of the c/a ratio from its ideal value. The Curie temperature in the MFA is slightly above the experimental value but a part of the difference can be ascribed to the MFA itself. The Curie temperatures can be neither expressed in terms of total energy differences between the AFM–FM states (or DLM–FM states) nor can they be obtained from the first nearest-neighbour interactions only. We investigated the structural sensitivity of the Curie temperature and found its strong dependence on the c/a ratio which can be related to the measured Curie temperatures of thick epitaxial Gd(0001) films on various transition-metal substrates. Analogous sensitivity of the exchange interactions and the Curie temperature was found on changing the hcp lattice to a hypothetical fcc structure. An improved estimation of the Curie temperature from the calculated exchange interactions as well as a comparison of theoretical and experimental magnon spectra are left for future studies.

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