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Exchange interactions in paramagnetic amorphous and disordered crystalline CrN-based systems

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We present a first principles supercell methodology for the calculation of exchange interactions of magnetic materials with arbitrary degrees of structural and chemical disorder in their high temperature paramagnetic state. It is based on a projection of the total magnetic energy of the system onto local pair clusters, allowing the interactions to vary independently as a response to their local environments. We demonstrate our method by deriving the distance dependent exchange interactions in vibrating crystalline CrN, a $\text{Ti}_{0.5}\text{Cr}_{0.5}\text{N}$ solid solution as well as in amorphous CrN. Our method reveals strong local environment effects in all three systems. In the amorphous case we use the full set of exchange interactions in a search for the noncollinear magnetic ground state.

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The understanding and accurate modeling of magnetic materials at finite temperatures is a grand challenge in solid state physics.¹ Its importance is highlighted by demands for new iron-based materials in the steel industry, improvements in materials for electrical motors and generators, and the outlook of the full utilization of the spin degree of freedom in electronics.^{2,3} The difficulties in providing an accurate description of high-temperature magnetic materials stem from the complexity of the quantum excitations that must be included in the models and simulations. Such excitations are of electronic, magnetic, vibrational, and structural nature with unknown individual impact.

Particularly, the treatment of amorphous magnets is problematic, as the lack of crystal symmetry hampers both experimental characterization as well as drastically increases computational costs in the theoretical approaches.^{4,5} Furthermore, the topological disorder is likely to induce unintuitive noncollinear magnetic configurations and methodological development is needed to understand their excitations.

In crystalline cases, one key approach to get around the quantum complexity has been the mapping of the magnetic configurational degree of freedom onto a semiclassical model Hamiltonian such as the Heisenberg model known for its applicability on systems with robust local moments. This model Hamiltonian,

$$\mathcal{H} = - \sum_{i \neq j} J_{ij} \mathbf{e}_i \cdot \mathbf{e}_j \quad (1)$$

where the J_{ij} 's are the magnetic exchange interactions (MEI) between pairs of magnetic atoms (i, j) and each $\mathbf{e}_i$ is a unit vector directed along the local atomic moment at site i , can subsequently be used in Monte Carlo⁶ or spin dynamics simulations^{7,8} to obtain critical temperatures for ordering (T_C), or to find ground state configurations.

This Heisenberg Hamiltonian, with only bilinear pair interactions, gives only an approximate description of the real complex magnetism in solid state systems. Its interactions correspond to the first terms of the complete expansion series of the magnetic configurational energy around the value of the fully disordered magnet. It neglects interactions corresponding to multisite clusters, biquadratic terms, and other higher

order terms in the expansion. Nevertheless, it has proven to be valuable in practice and is known to give an accurate description of the magnetic energies of several crystalline systems. Certainly, limitations of this magnetic Hamiltonian should be kept in mind.

Several mapping procedures based on first principles electronic structure calculations have been successfully employed to obtain the MEI. The perturbative magnetic force theorem proposed by Liechtenstein *et al.*^{9,10} has played an important role and has been implemented together with the disordered local moments (DLM)¹¹ treatment of paramagnetism in the generalized perturbation method (GPM).¹² Supercell approaches include the frozen magnon approach^{13,14} and the structure inversion methodology.¹⁵ Despite their success, all those methods suffer from difficulties to treat systems with arbitrary disorder as they, this far, have relied on the existence of an underlying lattice geometry. Hence, in our opinion, there is no established approach to obtain paramagnetic MEIs in systems with topological disorder, or even in configurationally disordered crystalline alloys with large local lattice relaxations. Moreover, the impact of temperature induced vibrations, the need to derive MEI from a disordered magnetic reference state,^{12,16} and local environment effects are often neglected.

In this work we propose a magnetic direct cluster averaging (MDCA) method, to calculate paramagnetic exchange interactions in a system with arbitrary geometry. The method is based on a conventional first principle supercell approach treating crystalline and noncrystalline materials on an equal footing. We illustrate the method for crystalline disordered rock-salt structure CrN and $\text{Ti}_{0.5}\text{Cr}_{0.5}\text{N}$ as well as amorphous CrN. The studied materials have attained substantial attention due to couplings between magnetic, electronic, and structural parameters with significant implications for technological applications.¹⁷⁻²¹ We also demonstrate that a benefit from the MDCA method is that it can be used as a baseline to ensure convergence within the Connolly-Williams (CW)²² structure inversion method.

The Hamiltonian in Eq. (1) describes both collinear and noncollinear magnetic configurations. Under the assumption that there are no important nonlinear higher order terms

present, such as the ones discussed in Ref. 23, the J_{ij} can be obtained from calculations restricted to collinear configurations. This observation is especially valid when the interactions in the high temperature paramagnetic state are desired, where the spin correlation functions are small, and one can follow the philosophy of the DLM approach.^{11,24} Thus, to obtain the exchange interactions we consider a system with a collinear magnetic configuration specified as $\sigma = \{\sigma_1, \sigma_2, \dots, \sigma_n\}$, where $\sigma_i \in \{\pm 1\}$ are spin variables for each site with a magnetic atom. This picture is equivalent to that of the configurational aspects of a binary alloy for which a general mathematical framework has been developed by Sanchez *et al.*²⁵ Following this analogy the magnetic interactions may be viewed as effective pair interactions in a cluster expansion procedure. However, since our aim is to calculate magnetic interactions in *disordered* systems, *where all pairs of atoms are unique*, we cannot rely directly on the traditional structure inversion approach, as it requires the presence of an underlying lattice symmetry to reduce the number of free fitting parameters. Instead we start with the very definition of the pair interactions as projections of the total energy, E , onto the cluster basis function of each individual pair of atoms. Accordingly, these projections define the exchange interactions, J_{ij}^* , as

$$J_{ij}^* = \frac{1}{N_{\sigma'}} \sum_{\sigma'} \left[-\frac{1}{8} \sum_{\sigma_i, \sigma_j = \pm 1} E(\{\sigma_i, \sigma_j\}; \sigma') \prod_{k=i,j} \sigma_k \right], \quad (2)$$

where the summation is performed over all possible configurations σ of N magnetic atoms divided in a summation over the configuration within the cluster $\{\sigma_i, \sigma_j\}$ and in the rest of the cluster denoted σ' . $N_{\sigma'} = 2^{(N-2)}$ is the total number of collinear magnetic configurations of the remaining $(N-2)$ sites. This procedure does have a counterpart in alloy theory that was suggested by Berera²⁶ and is referred to as direct cluster averaging (DCA). Here, we define the expression within the brackets of Eq. (2) as two-site magnetic potentials, according to

$$\begin{aligned} J_{ij}^{\sigma'} &= -\frac{1}{8} \sum_{\sigma_i, \sigma_j = \pm 1} E(\{\sigma_i, \sigma_j\}; \sigma') \prod_{k=i,j} \sigma_k \\ &= -\frac{1}{8} [E(\{\uparrow, \uparrow\}; \sigma') + E(\{\downarrow, \downarrow\}; \sigma') \\ &\quad - E(\{\uparrow, \downarrow\}; \sigma') - E(\{\downarrow, \uparrow\}; \sigma')]. \end{aligned} \quad (3)$$

We note that by including all the four energy terms in Eq. (3) the pair interaction between the moments on sites i and j is singled out as the effect of any other pair interaction between one of the moments within the cluster and any moment outside it is canceled. The averaging over the configurations σ' in Eq. (2) removes any possible effect of multisite interactions. In practical calculations, restrictions have to be imposed on the number of configurations that are considered, introducing an uncertainty in the values of J_{ij}^* . Thus, if we choose a subset of $N_{\zeta'}$ configurations $\{\zeta'\} \subset \{\sigma'\}$ randomly, we simultaneously obtain paramagneticlike configurations and allow for a treatment of the $J_{ij}^{\sigma'}$ as stochastic variables. Thus

we can estimate the MEI,

$$J_{ij}^* \approx J_{ij} = \frac{1}{N_{\zeta'}} \sum_{\sigma' \in \{\zeta'\}} J_{ij}^{\sigma'}, \quad (4)$$

with a confidence interval of degree $1 - \alpha$ with respect to the statistical sampling of magnetic configurations outside the pair: $J_{ij} - t_{\alpha/2}(f)d < J_{ij}^* < J_{ij} + t_{\alpha/2}(f)d$, where $t_{\alpha/2}(f)$ is a t distribution with $f = N_{\zeta'} - 1$ degrees of freedom and $d = s/\sqrt{N_{\zeta'}}$, where s is the estimated standard deviation of the J_{ij} . In this work we have used 95% confidence intervals plotted as error bars in the figures. The inset of Fig. 1 shows the individual two-site potentials [Eq. (3)] and the accumulated estimate of J_{ij}^* [Eq. (4)] for the case of nearest neighbor MEI in ideal CrN. In this case the set of configurations $\{\zeta'\}$ were based on 30 randomly generated supercells with an average spin correlation function on the first coordination shell as small as -0.006 .

The electronic structure problem was solved using density functional theory (DFT)^{27,28} and the projector augmented wave (PAW) method,²⁹ as implemented in the Vienna *ab initio* simulation package (VASP).^{30,31} To accurately describe strongly correlated Cr $3d$ electrons, the local spin density approximation with an additional Hubbard U term (LDA + U)^{32,33} of 3 eV was employed as discussed in detail in Ref. 24. 64 atom supercells were used for the derivation of nearest-neighbor (NN) interactions in CrN, while 96 atom cells were used to obtain next-NN interactions in CrN and the interactions in $\text{Ti}_{0.5}\text{Cr}_{0.5}\text{N}$. 250 atoms were used in the simulations of the amorphous CrN structure. The size of our calculation cells were carefully checked so that effects from interactions between periodic images were negligible.

The first application of the method is to investigate the influence of lattice vibrations on the magnetic exchange interactions. Figure 1 shows the calculated [Eqs. (3) and (4)] nearest-neighbor (NN) interactions in a realistic finite

FIG. 1. (Color online) Calculated magnetic exchange interactions on the first two Cr-Cr coordination shells of cubic CrN as a function of the interatomic distance. The values obtained from geometries derived with DLM-MD as well as idealized displacements of the atoms are shown. R_0^α is the equilibrium pair distance of the α th coordination shell ($\alpha = 1, 2$). The inset illustrates the application of Eqs. (3) and (4).

temperature geometry obtained in Ref. 34 by the disordered local moment molecular dynamics (DLM-MD) at 300 K. The figure shows interactions derived between the same pair of atoms at 16 different MD time steps, thus with different interatomic distances. To visualize the pure distance effect in $J_{ij}(|\mathbf{r}_i - \mathbf{r}_j|)$ we also calculated the values of the nearest- and next-nearest-neighbor interactions, when only the interaction pair was distorted from ideal lattice positions.

We observe a distinct dependency of the MEI on the distances between the atoms, even for slight deviations. The NN as well as the next-NN interactions are antiferromagnetic at zero deviation (-7.5 meV and -6.8 meV, respectively) with a sharp increase in antiferromagnetic (AFM) strength at smaller distances. However, when positioned far away, but still at a realistic distance as illustrated with presence in the MD data, the NN interaction actually does become positive. This qualitative difference between magnetic interactions induced by 300 K vibrations opens perspectives of phonon induced dynamic magnetic short range correlations in the paramagnetic state and, possibly, the opposite coupling depending on the magnetic and vibrational time scales.

The second application of the method is to study effects from substitutional chemical disorder in solid solutions. In such systems, different local chemical environments give rise to lattice relaxations and differences in the electronic structure of the magnetic components, and thus possibly differences in the exchange interactions. Such effects are, for instance, crucial to understand the INVAR effect in FeNi alloys.^{35,36}

Shown in Fig. 2 are the exchange interactions between a selection of Cr-Cr NN pairs on the metal fcc sublattice in a supercell model for the alloy $\text{Ti}_{0.5}\text{Cr}_{0.5}\text{N}$,³⁷ as a function of the interatomic distance in Å (top panel) and as a function of the number of Ti atoms that are NN to the pair (lower panel). The exchange interactions are generally ferromagnetic,

FIG. 2. (Color online) Magnetic exchange interactions between Cr-Cr pairs in a $\text{Ti}_{0.5}\text{Cr}_{0.5}\text{N}$ alloy as a function of the interatomic distances (top panel) and number of Ti nearest neighbors to the Cr-Cr pairs (lower panel). In the top panel the Ti rich environments are highlighted by open symbols and the values in pure CrN are included for comparison. In the lower panel, a linear regression trend line is provided as a guide for the eye.

in line with experiments^{38,39} but in sharp contrast to AFM CrN. Cr-Cr pairs with more than 10 NN Ti atoms seem to exclusively interact ferromagnetically. Thus the increasing presence of Ti atoms in the immediate surrounding of a Cr-Cr pair strongly influences their exchange coupling. This study reveals the importance of local environment effects on magnetic exchange interactions in these alloys, adding further complexity to the concentration dependence observed previously in this material.³⁷

The third application of our method is to study an extreme case of disorder in the form of topologically disordered amorphous CrN. We obtained our structural model for amorphous CrN by means of the stochastic quench method^{40,41} using 250 atoms in the supercell. To include the effect of temperature induced vibrations on the structure we first run 10 000 time steps of 1 fs by means of a standard quantum molecular dynamics method. The magnetic state was kept fixed and the temperature was 700 K, a typical growth temperature for amorphous nitride thin films.⁴² The QMD simulations are carried out using a canonical ensemble (NVT), neglecting thermal expansion. In order to maintain the temperature and avoid artificial energy drift we use the standard Nosé thermostat⁴³ implemented in VASP, with the Nosé mass corresponding to a 40 time step period. Then we run 1400 time steps of 1 fs of DLM-MD³⁴ at 300 K to average out any possible memory effects of specific magnetic orientations in the geometry.

The top panel of Fig. 3 shows the obtained Cr-Cr radial distribution functions (RDF) for our amorphous model as well as for our crystalline cubic CrN model after the MD simulation, both convoluted with a 0.2 Å Gaussian. The first peak of the a-CrN Cr-Cr RDF is at slightly lower distances as compared to c-CrN as several of the Cr atoms in the a-CrN case are positioned in a N-poor local environment allowing for smaller Cr-Cr distances. However, the volume of a-CrN is as expected larger than c-CrN.

FIG. 3. (Color online) Cr-Cr radial distribution function for the amorphous CrN model (a-CrN) compared to crystalline cubic CrN (c-CrN) (top panel) and the magnetic exchange interactions (lower panel) in the amorphous cell obtained with MDCA and MCW approaches, respectively. The inset in the lower panel is a zoom in of the short distance interactions comparing the MDCA results with the same interactions obtained with MCW.

In our supercell approach, we first investigated the range of the magnetic interactions. This was achieved by using the MDCA approach to calculate a subset of 20 chosen interactions out of the more than 4000 unique Cr-Cr pairs in our cell that has distances less than half of the supercell periodicity. We found that Cr-Cr pairs with larger separations than 5 Å have negligible interaction strengths of at most 1 meV, a value which is within our statistical error bars. This distance corresponds roughly to that of the third metal coordination shell in a CrN crystal. Thus we could focus on the 1456 Cr-Cr pairs with interatomic distances less than 5 Å, in our supercell of size 13.603 Å.

In the lower panel of Fig. 3 we show 127 exchange interactions obtained with our MDCA method. Our approach gives swift access to any chosen individual pair interaction, but if all the thousands of interactions in the amorphous supercell are desired, the method is computationally cumbersome. However, the initial MDCA survey of the J_{ij} 's has revealed both the relevant cutoff and provided a substantial subset of reliable interaction values. This translates into both a necessary limitation of the number of free parameters and a reliable convergence criteria to attempt a brute force CW structure inversion. Thus we performed a structure inversion using the 1456 J_{ij} 's within the 5 Å cutoff as independent free fitting parameters and gradually increased the included number of first-principles calculations of the energies of cells with random generated configurations σ in the procedure. We found that when the number of considered configurations was 4000, the values of the MEI had converged to the MDCA obtained values, with a mean absolute deviation of only 1.6 meV. The good agreement between the two methods is illustrated in the inset in Fig. 3. The MEI in amorphous CrN are predominantly AFM, especially at short distances, but at larger distances a fraction are ferromagnetic (FM). For all pair distances the spread in MEI is huge, underlying the need to treat all pair interactions as independent in any quantitative modeling scheme of amorphous magnets.

The obtained full set of exchange interactions up to $|\mathbf{r}_i - \mathbf{r}_j| = 5$ Å were then used in the noncollinear Heisenberg Hamiltonian in Eq. (1). We minimized the magnetic energy with respect to noncollinear configurations using a simulated annealing procedure with a Metropolis-type Monte Carlo simulation.⁴⁴ The energy was minimized in a $4 \times 4 \times 4$ supercell of our amorphous structure model, including 8000 Cr magnetic moments coupled by the calculated exchange interactions. The system was initiated in a disordered noncollinear spin configuration followed by a gradual decrease in temperature with 100 000 random trial spin rotations each temperature step. The procedure was initiated at several different starting temperatures in the interval 1000–100 K. The lowest energy state found was a noncollinear AFM configuration with a ferromagnetic component no larger than $0.01\mu_B$ per Cr atom. It was obtained for runs with starting temperatures in the range 200–100 K.

In conclusion, we demonstrate the vital importance of local environment effects on the magnetic exchange interactions in disordered systems, including amorphous magnets. For this purpose we have suggested a supercell technique inspired by the direct cluster averaging method from alloy theory, which could be fruitfully combined with a structure inversion approach. Our work opens up for theoretical predictions of ground state ordering and finite temperature magnetism in amorphous systems, as well as simulations of vibrational and configurational local environment effects on magnetism in alloys and compounds.

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