Fig. 1 show the pressure dependencies of the bulk moduli. With correct treatment of magnetism, one sees the expected small and gradual increase with pressure, contrary to the main conclusion made in ref. 1. An improved treatment of the correlation effects in the LDA+U model (with U = 4 eV) compared with the GGA does not result in any qualitative change, although it clearly improves the quantitative agreement with the experimental volumes.

Our *ab initio* calculations do not support the conclusions made by Rivadulla *et al.* for a collapse in the bulk modulus of CrN upon the cubic-to-orthorhombic transition. Further experimental and theoretical studies will be needed to clarify the origin of the apparent discrepancy between the theory and experimental indications in ref. 1. ❐

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Rivadulla *et al.* reply: Alling *et al.* suggest that our report of the reduction of the bulk modulus (K_0) at the structural phase transition in CrN is due to an incorrect assumption in our calculations. First, we would like to remark that our report is based on both experimental observations and *ab inito* calculations. Although the structural transition at room temperature occurs at too low a pressure to derive an accurate value of K_0 from the volume–pressure (V–P) fittings in the cubic phase, we do present in the supporting information experimental measurements of the dynamic Young modulus and internal friction. Both magnitudes are consistent with a strong suppression of K_0 in the orthorhombic (antiferromagnetic; AF) phase with respect to the cubic (paramagnetic; PM) phase. These are direct measurements that do not require any further manipulation of the data or fitting to any model.

Regarding the *ab initio* calculations, Alling *et al.* propose that the use of disordered local moments is crucial to reproduce the results for K_0 in the cubic phase, and that our approach of using a non-magnetic phase is inappropriate. They have used a unit cell with only 48 Cr atoms (roughly corresponding to a cube with a 9.8 Å lattice parameter). Their claim is that they can impose a random distribution of moments that would mimic the PM state observed in nature when sufficient thermal agitation is present. In this model, however, they can only impose two directions in spin space (up/down). Given the small number of atoms considered, this cannot be considered to be an accurate description of the random moment distribution that occurs in the presence of thermal agitation in a PM phase. Instead, the situation reproduced in their calculations describes some kind of AF ordering (probably short-ranged), not a real PM phase.

Alling *et al.* also claim that our scheme is incorrect because it does not lead to a gap opening around the Fermi level. We completely disagree with this comment. A gap opening is not obtained in any of our structural calculations using only the generalized gradient approximation (GGA), nevertheless, it is well known that the GGA alone can give an accurate description of the structural properties of this type of system with moderately correlated electrons. The introduction of the LDA+U scheme, which leads to a correct insulating state with a reasonable value of U, does not improve the lattice parameter or bulk modulus obtained, as Alling *et al.* show from their calculations. Thus, this would not be a reason to discard the use of a non-magnetic calculation to model the PM phase; the gap opening, by itself, does not lead to an improvement in the calculations of structural properties.

We would also like to remark that in the AF ordered phase, it is possible to compare directly experiment and theory by imposing a well-ordered AF state in our calculations. A good agreement is found between calculations and experiments in this case. Other magnetically ordered phases would give a value of K_0 closer to that obtained in the experimental AF phase, for example, in the short-ranged AF phase proposed by Alling *et al.* However, similar results (K_0 = 255 GPa) are also obtained for an AF structure different from that observed experimentally, but imposed with the same unit cell. In our opinion, these results are consistent and further indicate that the phase suggested by Alling *et al.* better represents some kind of magnetically ordered phase rather than a paramagnetic one.

Finally, in our paper we explain how the change in bonding takes place when net magnetism is absent in the crystal, compared with the magnetically ordered state. The charge accumulation along the Cr–Cr bonds when magnetism appears is crucial in determining the compressibility of the material, as we thoroughly discuss in the paper. All the results we present are in agreement with the model we propose in terms of bond changes that are reflected in a change in the bulk modulus, that is, the fact that magnetic coupling leads to a stronger Cr–Cr bond and weaker Cr–N bonds, with the corresponding reduction in bulk modulus in the magnetic phase, compared with the more covalent paramagnetic/non-magnetic phase. ❐

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