

**Elastic properties of fcc Fe-Mn- $X$  ( $X$ =Cr, Co, Ni, Cu) alloys from first-principles calculations**S. Reeh,<sup>1,\*</sup> D. Music,<sup>1</sup> M. Ekholm,<sup>2,3</sup> I. A. Abrikosov,<sup>2</sup> and J. M. Schneider<sup>1</sup><sup>1</sup>*Materials Chemistry, RWTH Aachen University, D-52056 Aachen, Germany*<sup>2</sup>*Department of Physics, Chemistry and Biology, Linköping University, SE-58183 Linköping, Sweden*<sup>3</sup>*Swedish e-Science Research Centre (SeRC), Linköping University, SE-58183 Linköping, Sweden*

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The influence of the valence electron concentration of  $X$  in fcc Fe-Mn- $X$  ( $X$ =Cr, Co, Ni, Cu) alloys on the elastic and magnetic properties has been studied by means of *ab initio* calculations for alloy element concentrations of up to 8 at. %  $X$ . We observe that Cu increases the bulk-to-shear modulus ( $B/G$ ) ratio by 19.2%. Simultaneously magnetic moments of Fe and Mn increase strongly. The other alloying elements induce less significant changes in  $B/G$ . The trends in  $B/G$  may be understood by considering the changes in  $G$  induced by the variation in valence electron concentration (VEC). As the VEC is increased, more pronounced metallic bonds are formed, giving rise to smaller shear modulus values. The changes in magnetic moments may be explained by the magnetovolume effect. Alloys with smaller VEC as Fe-Mn exhibit a decrease in local magnetic moments and equilibrium lattice parameters, while alloys with larger VEC as Fe-Mn demonstrate an increase in local magnetic moments and equilibrium lattice parameters. These data provide the basis for the design of Mn-rich steels with enhanced elastic properties.

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**I. INTRODUCTION**

High-Mn steels with a concentration of  $\sim 24$  at. % Mn exhibit extraordinary mechanical properties: high strength ( $>1000$  MPa) and high ductility (elongation to failure of  $>50\%$ ), which makes these steels very interesting for automotive applications.<sup>1</sup> These outstanding properties are based on two main deformation mechanisms, namely transformation induced plasticity (TRIP effect) and twinning induced plasticity (TWIP effect), during deformation.<sup>2</sup> The deformation mechanisms are influenced by the stacking fault energy (SFE). Frommeyer *et al.*<sup>2</sup> reported that with  $SFE < 16$  mJ/m<sup>2</sup> the TRIP effect is sustained and with  $SFE > 25$  mJ/m<sup>2</sup> the TWIP effect is favored. For fcc Fe-Mn alloys the SFE is dependent, *inter alia*, on the chemical composition.<sup>3</sup> It has recently been suggested that adding other transition metal elements such as Cr, Co, Ni, and Cu can be used to alter the SFE. Dumay *et al.*<sup>4</sup> calculated that the SFE is decreased by alloying with Cr and therefore martensite formation is sustained during deformation. For Cu Dumay *et al.*<sup>4</sup> predicted an increase of the SFE which would result in mechanical twinning. Ishida and Nishizawa<sup>5</sup> reported an increasing SFE for Ni and a decreasing SFE for Co additions at 300 K.

Pugh<sup>6</sup> suggested that macroscopic properties such as fracture strength of polycrystalline metals and resistance to plastic deformation are often related to elastic moduli such as the bulk modulus ( $B$ ) and shear modulus ( $G$ ). Moreover, the bulk-to-shear ratio ( $B/G$ ) was found to correlate with the ductility/brittleness crossover.<sup>6</sup> High values of  $B/G$  ( $>1.75$ ) are associated with ductility, while low values infer brittleness.<sup>6,7</sup> The  $B/G$  ratio has previously been employed by Vitos *et al.*<sup>7</sup> as a design criterion in predictive studies of austenitic stainless steels based on *ab initio* calculations.

In this work, we perform *ab initio* calculations based on density functional theory to systematically study the influence of changes in valence electron concentration (VEC) induced by additions of Cr, Co, Ni, and Cu on the elastic properties of high-Mn steels. We consider fcc Fe-Mn- $X$  ( $X$ =Cr, Co, Ni,

Cu) random alloys with an addition of  $X$  up to 8 at. % for two different Fe/Mn ratios of 2.33 and 4, and study in particular the VEC induced changes in  $B/G$  ratio and the local magnetic moments.

**II. COMPUTATIONAL DETAILS**

We have used the scalar-relativistic implementation of the exact muffin tin orbitals (EMTO) formalism<sup>8,9</sup> in combination with the full charge density (FCD) method<sup>10</sup> provided in the EMTO5.7 package. The EMTO method is based on the screened Korringa-Kohn-Rostocker Green's function method.<sup>11</sup> We used a  $13 \times 13 \times 13$   $k$ -points mesh to sample the Brillouin zone. In the self-consistency cycle, the core states were kept fixed (frozen-core approximation), and the total energy was converged within  $10^{-7}$  Ry. As in previous studies,<sup>12–14</sup> we use the local spin density approximation (LSDA) in the self-consistency cycle and evaluate total energy with the generalized gradient approximation (GGA) by Perdew-Burke-Ernzerhof (PBE).<sup>15</sup> Magnetic moments are also evaluated based on the LSDA charge density. This scheme improves the overestimation of magnetic moments of the PBE-GGA,<sup>16</sup> while leading to very similar values of the lattice constants in FeNi (Ref. 17) and FeMn (Ref. 18) systems as fully self-consistent GGA. Based on previous supercell calculations<sup>18</sup> we consider local lattice relaxations in this system to be of minor importance for this study. We therefore model the alloy potential by the coherent potential approximation (CPA),<sup>19,20</sup> which is an efficient tool to handle chemical as well as magnetic disorder. The reliability of the whole computational scheme for the FeMn system was studied in detail by Ekholm and Abrikosov.<sup>18</sup>

The magnetic state has been shown to have a crucial impact on ground-state properties of FeMn alloys.<sup>12,18,21–23</sup> In addition, finite temperature magnetic excitations have been demonstrated to be of great importance in transition metals<sup>24</sup> and their alloys, even below the magnetic ordering temperature.<sup>25</sup> Thus, quantum mechanically guided alloy

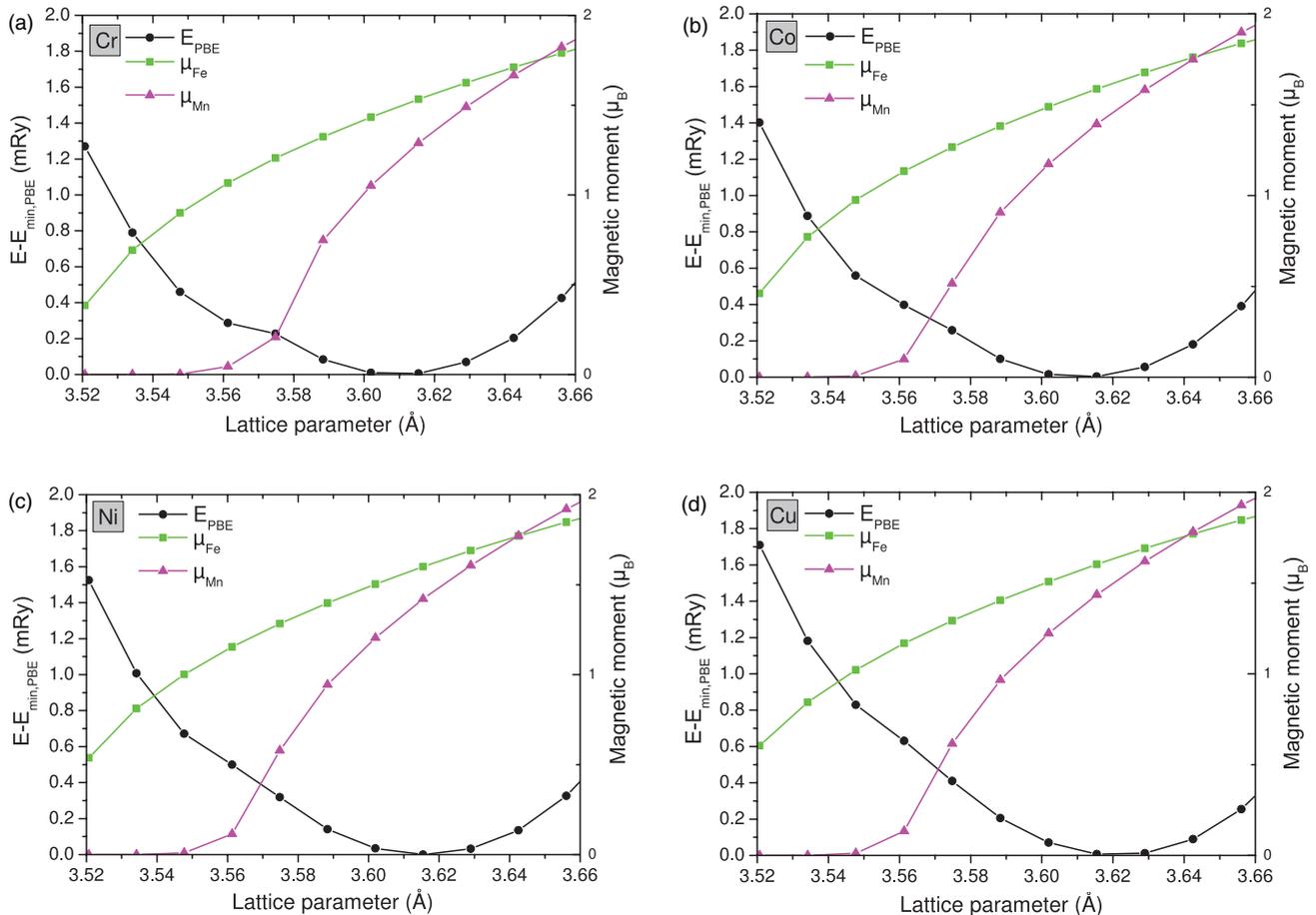


FIG. 1. (Color online) Total energy with respect to the minimum energy (dots) and local magnetic moments of Fe (rectangles) and Mn (triangles) versus lattice parameter calculated for Fe-Mn- $X$  with a Fe/Mn ratio of 2.33 and 2 at. %  $X$ , (a)  $X$ =Cr, (b)  $X$ =Co, (c)  $X$ =Ni, (d)  $X$ =Cu.

design strategies have to be based on a sound description of the magnetism of these alloys.<sup>12</sup>

Previous work on the FeMn system<sup>12,14,21</sup> based on the EMT method in combination with the frozen-core approximation has shown that the room temperature lattice constant and bulk modulus can be reproduced with good accuracy by describing the magnetic state with the disordered local moment (DLM) model. We therefore consider this computational method a suitable tool to guide high-throughput experimental work by parameter-free and internally consistent calculations. Details on the calculations of the elastic constants are described by Music *et al.*<sup>21</sup>

### III. RESULTS AND DISCUSSION

In Figs. 1(a)–1(d) the total energy with respect to the minimum energy and the local magnetic moments of Fe and Mn for fcc Fe-Mn- $X$  ( $X$ =Cr, Co, Ni, Cu) with a Fe/Mn ratio of 2.33 and an addition of 2 at. %  $X$  are plotted as a function of lattice parameter. For all  $X$  elements a transition between low-spin (LS) and high-spin (HS) magnetic states can be observed around 3.57 Å. Because the high-spin state has the lowest energy in all cases, only total energy data calculated after the transition point, i.e., in the HS state, were taken into account when determining the equilibrium lattice parameter

and the bulk modulus for each composition. We used the modified Morse equation of state.<sup>26,27</sup>

In Fig. 2 the calculated bulk and shear moduli of binary fcc Fe-Mn and ternary fcc Fe-Mn- $X$  ( $X$ =Cr, Co, Ni, Cu) for two Fe/Mn ratios 4 and 2.33 are shown. Here it is important to point out that due to the above mentioned HS to LS transition and the necessity to exclude the points for the LS solution from fitting the total energy, the calculated results for the bulk moduli turn out to be more noisy, compared to those for the shear moduli. Indeed, the latter are determined by volume-conserving distortions, and therefore are not directly affected by the magnetovolume effect.

Table I contains all VEC values for fcc Fe-Mn- $X$  ( $X$ =Cr, Co, Ni, Cu) alloys. It is clear that VEC is affected by  $X$ . For instance, the VEC value increases from 7.564 to 7.964 electrons per atom for the largest  $X$  concentrations in Fe-Mn- $X$  alloys with a Fe/Mn ratio of 2.33 as Cr is replaced with Co, Ni, and further with Cu. As the atomic concentration may be more useful for future experiments with these alloys than VEC, we consistently plot all figures and carry out discussions in these terms. All macroscopic observables, such as bulk and shear moduli as discussed below, may thus be related to VEC.

From Fig. 2 we conclude that within the above discussed noise, the bulk moduli appear to increase moderately for all the  $X$  additions to Fe-Mn. With addition of 8 at. %  $X$  the

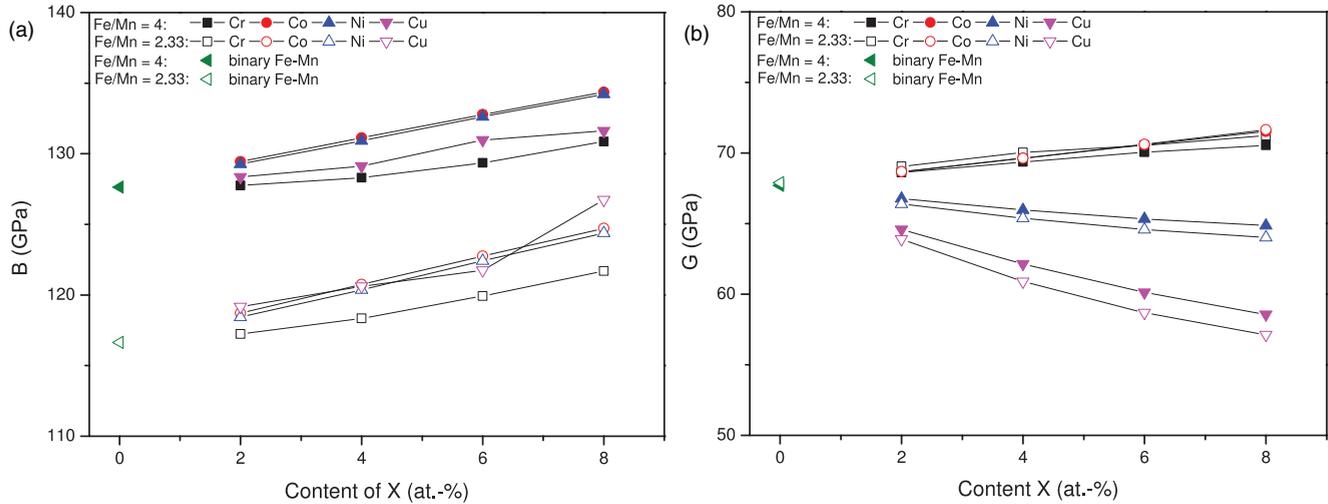


FIG. 2. (Color online) Bulk modulus (a) and shear modulus (b) for fcc Fe-Mn and Fe-Mn-X (X=Cr, Co, Ni, Cu) with an addition of X up to 8 at. % for Fe/Mn ratio=4 and 2.33.

increase in bulk modulus is with 6.5% the largest for Co. On the other hand VEC induced changes in shear modulus, which are determined after the Hill method,<sup>28</sup> are larger. Interestingly, while alloying with Cr and Co increases  $G$ , additions of Ni and Cu clearly decrease it. The largest effect is observed for an addition of 8 at. % Cu of a decrease of 15.6% and 18.9% with an addition of 8 at. % for a Fe/Mn ratio of 4 and 2.33, respectively. Thus, the shear modulus values show a decreasing trend when alloying with Ni and Cu which exhibit a larger VEC as Fe-Mn. Additions of Cr on the other hand showing a smaller VEC as Fe-Mn result in increased shear modulus values.

The dependence of the local magnetic moments  $\mu_{Fe}$  and  $\mu_{Mn}$  on the chemical composition is shown in Fig. 3. Within the DLM model, which we use to simulate the paramagnetic alloy, the local magnetic moments for all  $X$  elements in Fe-Mn- $X$  remain zero at equilibrium volume. However, the influence of the here investigated alloying elements  $X$  on the magnetic moments of Fe and Mn is substantial. With addition of Cu the local magnetic moment of Fe increases by 18% for a Fe/Mn ratio of 2.33 and 15% for a Fe/Mn ratio of 4. The effect of Cu on  $\mu_{Mn}$  is even larger: +46% for a Fe/Mn ratio of 2.33 and +34% for a Fe/Mn ratio of 4. The alloying with Ni shows the same trend as Cu:  $\mu_{Fe}$  increases with addition

of 8 at. % Ni by 13% and 10% for the Fe/Mn ratio of 2.33 and 4, and  $\mu_{Mn}$  is raised by 30% and 22%, respectively. The effect of Cr is inverse, as the local magnetic moments are decreased for both Fe and Mn. For a Fe/Mn ratio of 2.33  $\mu_{Fe}$  decreases with addition of 8 at. % Cr by 11% and  $\mu_{Mn}$

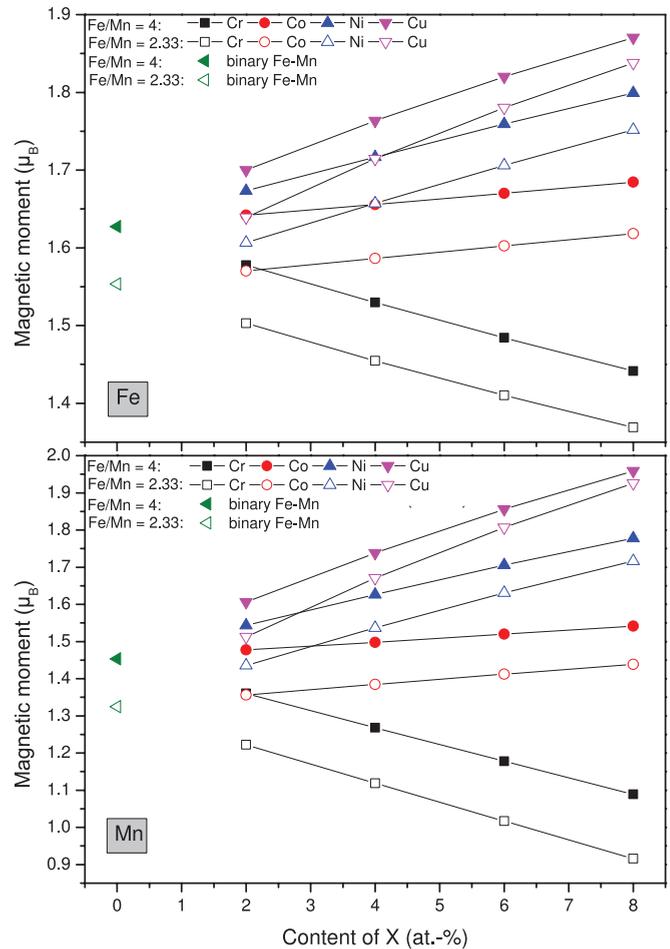


FIG. 3. (Color online) Local magnetic moments of Fe and Mn for fcc Fe-Mn-X (X=Cr, Co, Ni, Cu) with Fe/Mn ratio of 4 and 2.33.

TABLE I. Valence electron concentration (VEC, units are electrons per atom) for all concentrations of  $X$  in fcc Fe-Mn- $X$  alloys (X=Cr, Co, Ni, Cu) with Fe/Mn ratios of 2.33 and 4.

|            |    | Fe-Mn-X with additions of X in at. % |       |       |       |       |   |
|------------|----|--------------------------------------|-------|-------|-------|-------|---|
|            |    | X                                    | 0     | 2     | 4     | 6     | 8 |
| Fe/Mn=2.33 | Cr | 7.700                                | 7.666 | 7.632 | 7.598 | 7.564 |   |
|            | Co | 7.700                                | 7.726 | 7.752 | 7.778 | 7.804 |   |
|            | Ni | 7.700                                | 7.746 | 7.792 | 7.838 | 7.884 |   |
|            | Cu | 7.700                                | 7.766 | 7.832 | 7.898 | 7.964 |   |
| Fe/Mn=4    | Cr | 7.800                                | 7.764 | 7.728 | 7.692 | 7.656 |   |
|            | Co | 7.800                                | 7.824 | 7.848 | 7.872 | 7.896 |   |
|            | Ni | 7.800                                | 7.844 | 7.888 | 7.932 | 7.976 |   |
|            | Cu | 7.800                                | 7.864 | 7.928 | 7.992 | 8.056 |   |

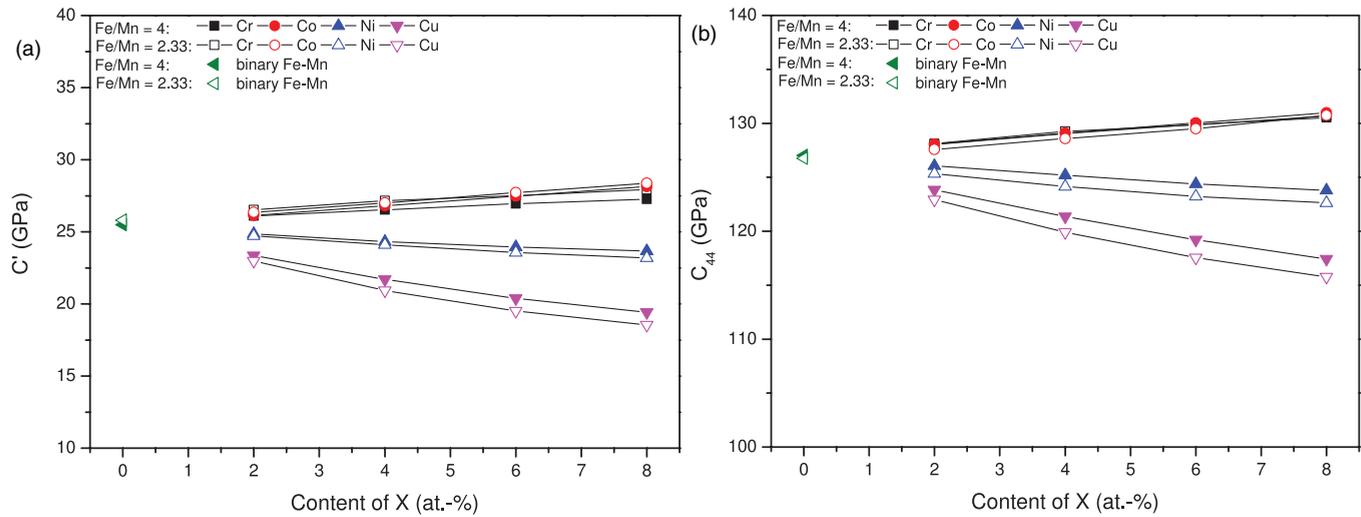


FIG. 4. (Color online) The shear moduli  $C'$  (a) and  $C_{44}$  (b) as function of concentration for fcc Fe-Mn and Fe-Mn-X ( $X=Cr, Co, Ni, Cu$ ) with an addition of X up to 8 at. % for Fe/Mn ratio=4 and 2.33.

decreases by 30%. For the Fe/Mn ratio of 4 the trend is similar:  $\mu_{Fe}$  and  $\mu_{Mn}$  decrease by 12% and 25%, respectively. With the addition of Co only marginal effects are observed. In general, a pronounced effect of the VEC on the local magnetic moments is observed. Alloys with smaller VEC as Fe-Mn exhibit a decrease in local magnetic moments, while alloys with larger VEC as Fe-Mn demonstrate an increase in local magnetic moments. The changes in the local magnetic moments may be explained with the magnetovolume effect.<sup>29</sup> The magnetic moments are coupled with the volume: The effect for the calculated equilibrium lattice parameter  $a_0$  is similar to the local magnetic moments for all additions of X in Fe-Mn-X alloys. Additions of Cr, which exhibit a smaller VEC as Fe-Mn, decrease  $a_0$  by 0.22% with 8 at. % Cr for a Fe/Mn ratio of 4. If Co is added to Fe-Mn, the decrease in lattice parameter is 0.11% for the same alloy. For additions of 8 at. % Ni and Cu, which show a larger VEC as Fe-Mn,  $a_0$  is increasing by 0.22% and 0.74% for a Fe/Mn ratio of 4, respectively.

Figure 4 displays the calculated shear moduli  $C'$  and  $C_{44}$  as a function of concentration X for two Fe/Mn ratios 4 and 2.33 for the binary and the ternary alloys. Both elastic constants show a decreasing trend with increasing VEC of the alloying element. Additions of Cu result in the largest decrease for both moduli and for both Fe/Mn ratios. Alloys with 8 at. % Cu cause a decrease of 31.3% and 39.2% for  $C'$  and 8.2% and 9.5% for  $C_{44}$  for the Fe/Mn ratios of 4 and 2.33, respectively. Since  $C_{44}$  has the largest effect on the shear modulus G, these trends are consistent with the trend showed in Fig. 2(b).

The  $B/G$  ratio for the fcc Fe-Mn-X ( $X=Cr, Co, Ni, Cu$ ) with Fe/Mn ratio of 4 and 2.33 is plotted in Fig. 5. For comparison with other fcc phases, the  $B/G$  ratios of both pure Cu, Ni, and Ir (Refs. 30 and 31) and two Fe-Cr-Ni-Mn alloys<sup>32</sup> are added. These reference compounds were chosen since they are isostructural to Fe-Mn-X. For both Fe/Mn ratios the  $B/G$  ratio is strongly increasing with addition of Cu (19.2% increase at Fe/Mn ratio 2.33 and 11.4% increase at Fe/Mn ratio 4 for 8 at. % Cu additions). With addition of 8 at. % Ni the  $B/G$  ratios are increased by 11.6% and 8.9% for

both Fe/Mn ratios studied here, respectively. For Co and Cr the  $B/G$  ratio is only marginally affected by composition. The observed trend follows directly from the individual behavior of B and G for the considered alloys. Indeed, for Cr and Co additions both B and G increase, compensating each other's contributions to  $B/G$  ratio to a very large degree. On the contrary, for Ni, and especially Cu, B is slightly increasing, while G is decreasing significantly upon alloying. Consequently, we observe a relatively large increase of the  $B/G$  ratio, especially for Cu. Note that pure Cu is known to be ductile<sup>6,33,34</sup> exhibiting the highest  $B/G$  ratio<sup>30</sup> in comparison to the here investigated alloying elements, which is consistent with our data. The  $B/G$  ratio of Ni and the Fe-19Cr-3Ni-13Mn alloy is in the same range as the investigated alloys within this work.<sup>32</sup> Pure Ir possesses the lowest  $B/G$  ratio of 1.6 (Ref. 30) of all alloying elements considered here and can be characterized as brittle material.<sup>33,34</sup> Hence, the here studied

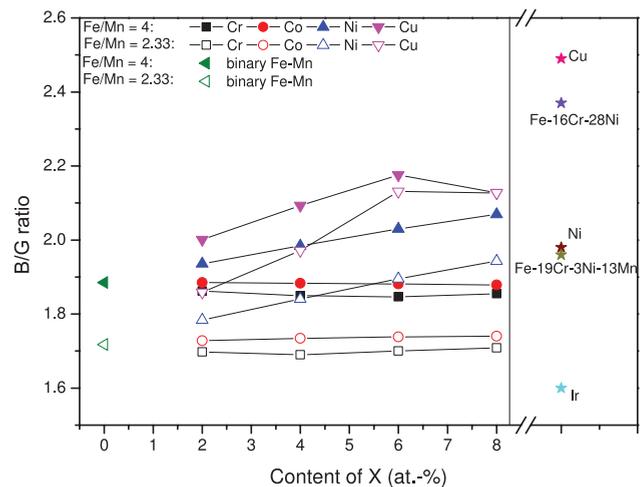


FIG. 5. (Color online) The calculated  $B/G$  ratio for fcc Fe-Mn-X ( $X=Cr, Co, Ni, Cu$ ) with Fe/Mn ratio of 4 and 2.33 in comparison with  $B/G$  ratio of other fcc phases.

Fe-Mn- $X$  alloys behave in a similar fashion regarding  $B/G$  as other fcc metals or alloys. In transition metal alloys with cubic crystal structure  $d$  orbitals with different symmetry,  $t_{2g}$  and  $e_g$ , have different spatial distributions. Ponomareva *et al.*<sup>35</sup> suggested that preferential occupation of  $t_{2g}$  or  $e_g$  orbitals leads to more directional bonding as compared to uniform occupation, as in Cu, which has a fully occupied  $d$  band. Thus, the materials with not fully occupied  $d$  bands should have a stronger covalent component in the bonding, and they should exhibit higher shear modulus values. For the pure elements Ir, Ni, and Cu the  $B/G$  ratio is indeed increasing with increasing VEC; more metallic bonds are formed, which is consistent with the trends observed for the alloys studied within this work. Fe-Mn alloys with additions of Cu exhibit the highest VEC and hence the largest  $B/G$  ratio. These Cu-based alloys seem to be the most ductile in comparison with other additions with Cr, Co, and Ni. In view of the fact that these high-Mn steels are interesting for automotive applications<sup>1</sup> a more enhanced ductility may play an important role in order to produce suitable car components in the process operations.

Figure 6 contains the total and partial density of states for Fe-Mn-Cr (VEC=7.564 electrons per atom), Fe-Mn (VEC=7.700 electrons per atom), and Fe-Mn-Cu (VEC=7.964 electrons per atom) for Fe/Mn ratio of 2.33 and  $X = 8$  at.%. It is evident that the metallic bonding character dominates in these alloys as the Fermi level is occupied, with the  $d$  states being the major contribution. The asymmetry between the spin-up and spin-down states leads to the composition dependence of the magnetic moments (see Fig. 3). The largest asymmetry is found for Fe-Mn-Cu giving rise to the largest magnetic moments. In all of these alloys the  $d$  states of Fe and Mn are not fully occupied. Cr induces even lower occupancies as it reduces the corresponding VEC. On the other hand, Cu increases the occupancy of the  $d$  band. This is consistent with the notion discussed above that the alloys with not fully occupied  $d$  band have a stronger covalent component and may thus exhibit higher shear moduli.

#### IV. CONCLUSION

The influence of the VEC of  $X$  in Fe-Mn- $X$  ( $X$ =Cr, Co, Ni, and Cu) on the  $B/G$  ratio and local magnetic moments was explored. Additions with Cr and Co seem to exhibit no substantial effect on the  $B/G$  ratio, while with additions of Cu and Ni the  $B/G$  ratio is increased up to 19.2% and 11.6%, respectively. The trends in  $B/G$  may be understood by considering the VEC induced changes in  $G$ . As the VEC is increased, more pronounced metallic bonds are formed, giving rise to smaller shear modulus values.

The local magnetic moments of Fe and Mn are decreased with additions of 8 at.% Cr by 30% and 12%, respectively. Alloys with Co do not affect the local magnetic moments significantly. Additions of Cu and Ni in Fe-Mn alloys result in an increase of the local magnetic moments of Fe and Mn: The strongest increase is observed for additions of Cu by +46% for  $\mu_{Mn}$  as well as +18% for  $\mu_{Fe}$ , while alloys with Ni show the same trend with a reduction of +30% for  $\mu_{Mn}$  as well as +13% for  $\mu_{Fe}$ . The changes in magnetic moments is caused by the magnetovolume effect.

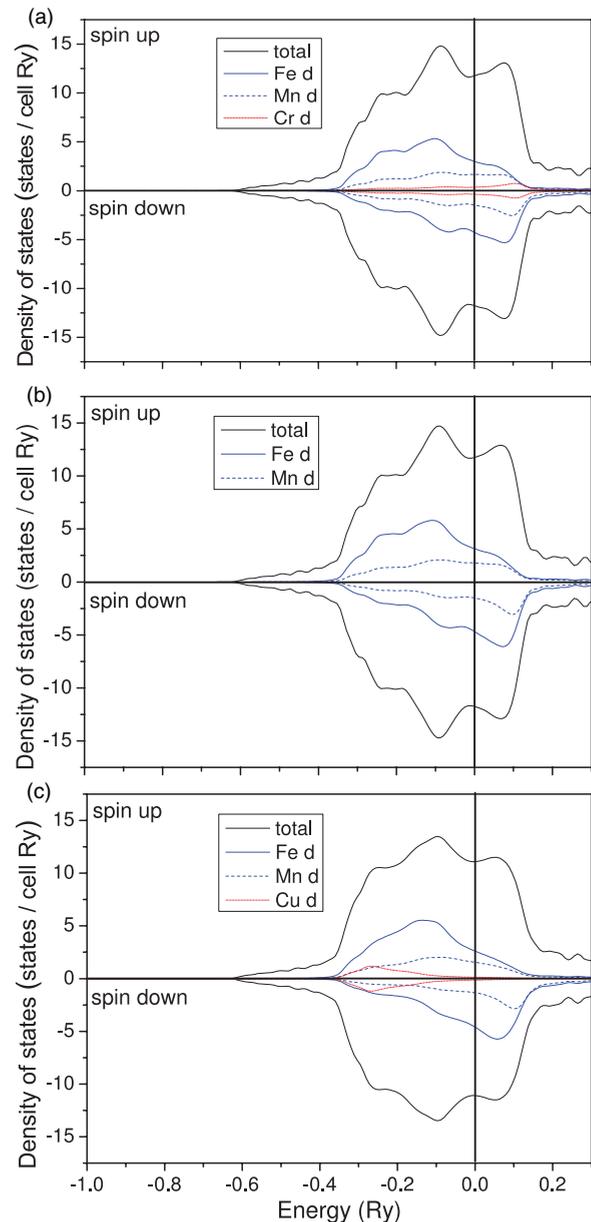


FIG. 6. (Color online) Total and partial ( $d$  bands) density of states for fcc Fe-Mn and Fe-Mn- $X$  ( $X$ =Cr, Cu) with Fe/Mn ratio of 2.33, where  $X = 8$  at.%. The Fermi energy is marked with a vertical solid line.

The equilibrium lattice parameter  $a_0$  is increased for Cu and Ni by 0.74% and 0.22% for an addition of 8 at.% Cu or Ni, respectively. Additions of Co cause, with  $-0.11\%$ , a minute reduction in lattice parameter. For additions of Cr the lattice parameter is decreased by 0.22% for 8 at.% Cr additions. These trends are consistent with the trends observed for the local magnetic moments. Alloying elements with smaller VEC as in Fe-Mn are characterized by decreased local magnetic moments and equilibrium lattice parameters, while alloying with elements with a larger VEC as Fe-Mn cause an increase in local magnetic moments and equilibrium lattice parameters. Hence, based on these calculations, with the  $B/G$  ratio as a design criterion, we propose in particular Cu as a promising alloying element for Fe-Mn alloys to increase the ductility significantly.

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- <sup>1</sup>O. Grässel and G. Frommeyer, *Stahl Eisen* **122**, 65 (2002).
- <sup>2</sup>G. Frommeyer, U. Brück, and P. Neumann, *ISI Int.* **43**, 438 (2003).
- <sup>3</sup>O. Grässel, L. Krüger, G. Frommeyer, and L. W. Meyer, *Int. J. Plast.* **16**, 1391 (2000).
- <sup>4</sup>A. Dumay, J. P. Chateau, S. Allain, S. Migot, and O. Bouaziz, *Mater. Sci. Eng. A* **483-84**, 184 (2008).
- <sup>5</sup>K. Ishida and T. Nishizawa, *Trans. Jpn. Int. Met.* **15**, 225 (1974).
- <sup>6</sup>S. F. Pugh, *Philos. Mag.* **45**, 823 (1954).
- <sup>7</sup>L. Vitos, P. A. Korzhavyi, and B. Johansson, *Phys. Rev. Lett.* **88**, 155501 (2002).
- <sup>8</sup>L. Vitos, *Phys. Rev. B* **64**, 014107 (2001).
- <sup>9</sup>K. Andersen, O. Jepsen, and G. Krier, *Lectures on Methods of Electronic Structure Calculations* (World Scientific, Singapore, 1994).
- <sup>10</sup>L. Vitos, J. Kollár, and H. L. Skriver, *Phys. Rev. B* **55**, 13521 (1997).
- <sup>11</sup>L. Vitos, H. L. Skriver, B. Johansson, and J. Kollár, *Comput. Mater. Sci.* **18**, 24 (2000).
- <sup>12</sup>T. Gebhardt, D. Music, M. Ekholm, I. A. Abrikosov, J. von Appen, R. Dronskowski, D. Wagner, J. Mayer, and J. M. Schneider, *Acta Mater.* **59**, 1493 (2011).
- <sup>13</sup>H. Zhang, M. P. J. Punkkinen, B. Johansson, and L. Vitos, *Phys. Rev. B* **85**, 054107 (2012).
- <sup>14</sup>T. Gebhardt, D. Music, B. Hallstedt, M. Ekholm, I. A. Abrikosov, L. Vitos, and J. M. Schneider, *J. Phys.: Condens. Matter* **22**, 295402 (2010).
- <sup>15</sup>J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).
- <sup>16</sup>A. V. Ruban and I. A. Abrikosov, *Rep. Prog. Phys.* **71**, 046501 (2008).
- <sup>17</sup>A. V. Ruban, S. Khmelevskiy, P. Mohn, and B. Johansson, *Phys. Rev. B* **75**, 054402 (2007).
- <sup>18</sup>M. Ekholm and I. A. Abrikosov, *Phys. Rev. B* **84**, 104423 (2011).
- <sup>19</sup>P. Soven, *Phys. Rev.* **156**, 809 (1967).
- <sup>20</sup>L. Vitos, I. A. Abrikosov, and B. Johansson, *Phys. Rev. Lett.* **87**, 156401 (2001).
- <sup>21</sup>D. Music, T. Takahashi, L. Vitos, C. Asker, I. A. Abrikosov, and J. M. Schneider, *Appl. Phys. Lett.* **91**, 191904 (2007).
- <sup>22</sup>N. I. Medvedeva, D. Van Aken, and J. E. Medvedeva, *J. Phys.: Condens. Matter* **22**, 316002 (2010).
- <sup>23</sup>I. A. Abrikosov, M. Ekholm, A. V. Ponomareva, and S. A. Barannikova, in *Magnetism and Magnetic Materials V*, Solid State Phenomena Vol. 190, edited by N. Perov and V. Rodionova (Trans Tech Publications Ltd, Stafa-Zurich, 2012), pp. 291–294.
- <sup>24</sup>T. Hickel, B. Grabowski, F. Körmann, and J. Neugebauer, *J. Phys.: Condens. Matter* **24**, 053202 (2012).
- <sup>25</sup>M. Ekholm, H. Zapolsky, A. V. Ruban, I. Vernyhora, D. Ledue, and I. A. Abrikosov, *Phys. Rev. Lett.* **105**, 167208 (2010).
- <sup>26</sup>V. L. Moruzzi, J. F. Janak, and K. Schwarz, *Phys. Rev. B* **37**, 790 (1988).
- <sup>27</sup>P. M. Morse, *Phys. Rev.* **34**, 57 (1929).
- <sup>28</sup>R. Hill, *Proc. Phys. Soc. London, Sect. A* **65**, 349 (1952).
- <sup>29</sup>M. van Schilfhaarde, I. A. Abrikosov, and B. Johansson, *Nature* **400**, 46 (1999).
- <sup>30</sup>C. Kittel, *Introduction to Solid State Physics* (Wiley, New York, 1996).
- <sup>31</sup>R. E. MacFarlane, J. A. Rayne, and C. K. Jones, *Phys. Lett.* **20**, 234 (1966).
- <sup>32</sup>S. Kim, H. Ledbetter, and Y. Y. Li, *J. Mater. Sci.* **29**, 5462 (1994).
- <sup>33</sup>T. Takahashi, R. Iskandar, F. Munnik, D. Music, J. Mayer, and J. M. Schneider, *J. Alloys Compd.* **540**, 75 (2012).
- <sup>34</sup>K. J. Van Vliet, J. Li, T. Zhu, S. Yip, and S. Suresh, *Phys. Rev. B* **67**, 104105 (2003).
- <sup>35</sup>A. V. Ponomareva, E. I. Isaev, Y. K. Vekilov, and I. A. Abrikosov, *Phys. Rev. B* **85**, 144117 (2012).