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The hyperfine properties of a hydrogenated Fe/V superlattice

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Abstract We study the effect of hydrogen on the electronic, magnetic and hyperfine structures of an iron-vanadium superlattice consisting of three Fe monolayers and nine V monolayers. The contact charge density (ρ), the contact hyperfine field (B_{hf}) and the electronic field gradient (EFG) at the Fe sites for different H locations and H fillings are calculated using the first principle full-potential linear-augmented-plane-wave (FP-LAPW) method. It is found that sizeable changes in the hyperfine properties are obtained only when H is in the interface region.

Keywords Hyperfine properties · Hydrogenated iron-vanadium · Superlattice

1 Introduction

Iron-vanadium superlattices constitute a benchmark for the various studies carried out on magnetic nanostructures. Due to the slight mismatch between the Fe and V lattice constants, the superlattices have tetragonal structures. The *c*/*a* ratio was found to depend on the thicknesses of Fe and V layers [1]. The quality of the Fe-V interface of dc sputtered samples was studied by Andersson et al. [2] using conversion electron Mössbauer spectroscopy (CEMS) and x-ray diffraction. Sharp interfaces were found for growth temperatures of 330°C or less. Large V induced magnetic moments for the trilayer V/Fe/V were obtained by Clavero et al. using a diverse assortment of experimental techniques [3]. From CEMS measurements by Nordström et al. [4], iron layers of thickness less than five monolayers were reported to be non-magnetic. Kalska et al., using CEMS, also reported differences in the degree of flatness between Fe on V and V on Fe interfaces [5].

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Introduction of H into Fe/V superlattices strongly distort the local lattice structure as determined through extended x-ray absorption fine structure, where variations up to around 7% of the local *c* parameter were reported [6]. Moreover, a hydrogen depletion zone of 1–2 monolayers in the V layer was reported [7]. The magnetic properties of Fe/V superlattices can be reversibly tuned by hydrogenation [8]. For a two-monolayer Fe superlattice, it was found that the Fe atoms in the pristine sample possess a magnetic moment of 1.7 μ_B, while for the hydrogenated samples the Fe atoms with neighboring V-H complexes possess moments in the range 2.1–2.2 μ_B [8]. The average magnetic moment per Fe atom was found to increase with increasing H content [9]. To our knowledge, there are no Mössbauer data on hydrogenated Fe/V superlattices.

The effect of H on the IEC and magnetic moment of a superlattice composed of three Fe layers and five V layers was studied by Ostanin et al. [10] using the full-potential linear-muffin-tin orbitals. The disappearance of the antiferromagnetic interlayer exchange coupling (IEC) for large H concentration was attributed to the decrease of the density of states at the Fermi level.

We used the FP-LAPW method as implemented in the WIEN2k package [11] to calculate the hyperfine properties at the interface and inner Fe sites in Fe_3V_9 superlattice versus the H location and H content. It is found that sizeable changes in the hyperfine properties are obtained only when H is in the interface region. The technical details of the calculation are found in [12] by Elzain and Al-Barwani.

2 Results and discussion

Figure 1 shows the unit cell along the BCC <001> direction used to calculate the magnetic and hyperfine properties of the hydrogenated Fe/V superlattice Fe_3V_9. We have performed calculations with H atoms at both Oz octahedral and tetrahedral interstitial sites. This paper shows the results with the H atoms at the Oz octahedral sites (Fig. 1). The H atoms are indexed by numbers from −1 to 5 with H at the interface Fe monolayer being indexed 0. Hydrogen atoms with index 5 lie at the centre of the V layer, while those with indices 1 and −1 lie at the V interface monolayer and the Fe interior monolayer respectively. The lattice parameters were relaxed to give the energy minimum. Ferromagnetic interlayer configurations were found to be energetically stable in all the present cases. In Table 1 we show the magnetic hyperfine fields (B_{hf}) at the interface and the central Fe monolayers together with the local Fe moments for different H locations. As seen from the table the values of B_{hf} for H locations farther from the interface remain almost the same as that of the H free case Fe_3V_9. The magnitudes of B_{hf} at both Fe sites for H at positions 1 and 0 at the interface are larger than that of Fe_3V_9. The corresponding local magnetic moments within the muffin-tin radii show almost similar trends. However, we find that the ratios of B_{hf} to the local moments of Fe at the two sites are different. It is clear that the effect of H on the magnetic hyperfine fields is felt only when the H atoms are located at the interface.

The isomer shifts at the interface and central Fe atoms relative to α-Fe are shown in Table 2. In general the values of the isomer shifts for H position far from the interface are small. Comparing the values of the isomer shifts to that of H free case (Fe_3V_9), sizeable changes are observed only when H is at the interface or inside

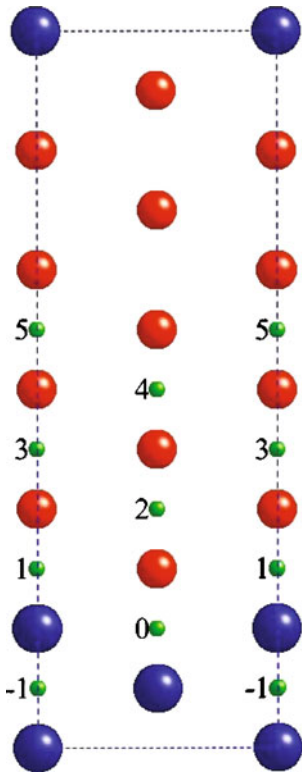

Fig. 1 Fig. 1 The unit cell of the Fe_3V_9 superlattice. Dark (*blue*) large balls represent Fe and light (*red*) large balls represent V. The small (*green*) balls represent H at the (Oz) octahedral interstitial sites. The indices give the hydrogen locations within the superlattice

Table 1 The first and second rows: the contact hyperfine fields (in Tesla) and the third and fourth rows: the local magnetic moments (in Bohr Magnetons) at the interface Fe (0), the interior Fe (−1) for different H locations

	Fe_3V_9	−1	0	1	2	3	4	5
Fe (0)	−17.5	−14.1	−22.0	−21.4	−17.5	−18.1	−18.3	−18.0
Fe (−1)	−22.0	−28.5	−25.8	−24.4	−22.0	−22.9	−23.0	−22.4
Fe (0)	1.57	1.57	2.03	1.86	1.63	1.63	1.59	1.54
Fe (−1)	2.55	2.59	2.42	2.54	2.58	2.54	2.56	2.55

the Fe layer. We found that the changes in the contact charge densities of Fe at the interface and the central sites follow the same trends as the change in atomic volumes at the same sites. This confirms our earlier conclusion that changes in the properties of Fe/V superlattices are attributed to volume effect [12].

The quadrupole splittings shown also in Table 2 are in general large at the Fe interface atom and relatively small for the central Fe atom. From these results one concludes that the effect of H outside the interface region can not be detected by the Mössbauer measurement.

We now consider the effect of H filling of the Oz sites starting from the center of the V layer and proceeding towards the interface. In Table 3 we show the magnetic hyperfine field, the isomer shift and the quadrupole splitting at the interface and the central Fe atoms versus the ratio of the number of H atoms to the number of V atoms

Table 2 The isomer (top) and quadrupole (bottom) splitting in mm/s at the interface Fe(0) and the central Fe(−1) atoms respectively for different H locations

	Fe_3V_9	−1	0	1	2	3	4	5
Fe (0)	−0.08	0.02	0.37	0.10	−0.07	−0.05	−0.04	−0.06
Fe (−1)	0.01	0.43	0.16	0.07	0.03	0.03	0.05	0.04
Fe (0)	−0.40	−0.40	−1.24	0.09	−0.33	−0.60	−0.32	−0.41
Fe (−1)	−0.05	−0.79	−0.09	0.09	−0.12	−0.05	−0.07	−0.06

Table 3 The respective magnetic hyperfine field (in Tesla, top), the isomer shift (in mm/s, middle) and the quadrupole splitting (in mm/s, bottom) at the interface Fe(0) and the central Fe(−1) atoms versus the fraction of H at the Oz sites

H/V	0	1/9	2/9	3/9	4/9	5/9
Fe (0)	−17.5	−18.0	−18.6	−18.9	−18.7	−18.5
Fe (−1)	−22.1	−22.4	−22.9	−22.9	−23.1	−23.6
Fe (0)	−0.08	−0.06	−0.05	−0.04	−0.04	−0.06
Fe (−1)	0.01	0.04	0.04	0.05	0.05	0.04
Fe (0)	−0.40	−0.41	−0.36	−0.34	−0.52	−0.59
Fe (−1)	−0.05	−0.06	−0.06	−0.10	−0.05	−0.05

in the unit cell. We note that the isomer shift does not practically change with H contents, while the magnitude of the magnetic hyperfine field at central monolayer slightly increases. The magnitude of the quadrupole splitting decreases at first and then increases as H contents increases.

As a result of these findings, when H is introduced in Fe/V superlattices there will be minor changes in the magnetic hyperfine fields and the quadrupole splitting at the Fe sites in the interface region if H is restricted to region outside the interface. This is in contrast with increase in the average magnetic moment with H contents observed experimentally [9] and confirmed theoretically [12]. However, the presence of H in the interface region will be reflected in large changes in all hyperfine parameters. Henceforth, Mössbauer measurements could be used to detect the absence or presence of H in the interface region.

In conclusion, the magnetic hyperfine fields, isomer shifts and quadrupole splittings at the interface and the central Fe sites in a Fe_3V_9 flat interface superlattice were calculated for different H locations and different H fillings. It is found that significant changes in the hyperfine parameters are detectable only when H resides in the interface region. This could be used to confirm the presence or absence of a depletion region in Fe/V superlattices.

References

1. Björck, M., Pärnaste, M., Marcellini, M., Andersson, G., Hjörvarsson, B.: J. Magn. Magn. Mater. **313**, 230 (2007)
2. Andersson, G., Nordström, E., Wäppling, R.: Eurphys. Lett. **60**, 731 (2002)
3. Clavero, C., Skuza, J.R., Choi, Y., Haskel, D., Sanchez-Hanke, C., Loloee, R., Zhernenkov, M.: Phys. Rev. B **80**, 024418 (2009)
4. Nordström, E., Kalska, B., Häggström, L., Blomqvist, P., Wäppling, R.: Hyperfine Interact. **141/142**, 465 (2002)
5. Kalska, B., Blomqvist, P., Häggström, L., Wäppling, R.: Europhys. Lett. **53**, 395 (2001)

6. Pálsson, G.K., Kapaklis, V., Dura, J.A., Jacob, J., Jayanetti, S., Rennie, A.R., Hjörvarsson, B.: Phys. Rev. B **82**, 245424 (2010)
7. Andersson, G., Hjörvarsson, B., Isberg, P.: Phys. Rev B **55**, 1774 (1997)
8. Remhof, A., Nowak, G., Zabel, H., Björck, M., Pärnaste, M., Hjörvarsson, B., Uzdin, V.: Europhys. Lett. **79**, 37003 (2007)
9. Labergerie, D., Westerholt, K., Zabel, H., Hjörvarsson, B.: J. Magn. Magn. Mater. **225**, 373 (2001)
10. Ostanin, S., Uzdin, V.M., Demangeat, C., Wills, J.M., Alouani, M., Dreyssé, H.: Phys. Rev. B **61**, 4870 (2000)
11. Blaha, P., Schwarz, K., Madsen, G.K.H., Kvasnicka, D., Luitz, J.: In: Schwarz, K. (ed.) WIEN2k: An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties. Technische Universitat Wien, Vienna, Austria (2009)
12. Elzain, M., Al-Barwani, M.: Mod. Phys. Lett. B **25**, 2239 (2011)