Abstract Submitted
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Structural and electronic origin of large magnetostrictive $Fe_{1-x}Ga_x$ alloys[1] HUI WANG, Shenyang National Laboratory of Materials Science, Institute of Metal Research and International Centre of Materials Physics, Chinese Academy of Scie, YANNING ZHANG, RUQIAN WU, LIZHI SUN, University of California, Irvine, SONSHENG XU, ZHIDONG ZHANG, Shenyang National Laboratory of Materials Science, Institute of Metal Research and International Centre of Materials Physics, Chinese Academy of Scie — $Fe_{1-x}Ga_x$ binary alloys exhibiting large magnetostriction and excellent ductility have great potentials for various applications. The origin of large magnetostriction has not been thoroughly studied, especially at high Ga concentration ($x > 18.75\%$). We conduct extensive ab initio molecular dynamics simulation of $Fe_{1-x}Ga_x$ alloys to generate atomic structures; and find that the alloys adopt the disordered A2 structure for $x < 18.75\%$ and the A2+$D0_3$ mixed structures for $18.75\% < x < 23.4\%$, respectively. The formation of $D0_3$-like structure play a key role for the decrease of magnetostriction beyond $x = 19\%$. Interestingly, the magnetostriction may greatly enhance, up to $\lambda_{001} = 850$ ppm in ternary alloys with incorporation of $3 - 5\%$ Cu and Zn.

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