STABILITY ANALYSIS OF DIFFERENT THIN MAGNESIUM NANOWIRES

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Abstract

Mg_n (n=1-5) nanowires of different isomeric structures have been investigated by employing ab-initio method. We have considered various geometrical structures up to five atoms to explore the global minimum energy configuration. The calculation of total energy, binding energy (B.E.), internal energy, band energy, Fermi energy, and density of states (DOS) have been carried out in large energy interval. We have analyzed the effect of shape and size on these calculated values and investigated DOS.

INTRODUCTION :

The metallic nanowires are attracting considerable attention because they represent a unique system for exploring phenomeno at the nanoscale and also due to their potential applications. Experimentally, Magnesium have been used as substrate material for different nanowire preparation. Xing *et al* [2] worked on the synthesis and characterization of $MgAl_2O_4$ spinal nanowires. Limin Cao *et al* [3].

RESULTS AND DISCUSSION:

The calculations have been performed using ABINIT code[4], which uses pseudopotential and the plane waves of the density functional theory. An efficient Fast Fourier Transform algorithm [5] is used for the conversion of the wave functions between the real and reciprocal lattices. The wave functions are determined in a fixed potential according to a state-by-state or band-by-band conjugate gradient algorithm [6, 7]. We have considered TM potentials [8]. First we consider the monoatomic linear chain having one Mg atom per unit cell. The binding energy so obtained is 3.16 eV/atom. For two atom Mg wire, we have examined three types of geometrical structure i.e. linear, ladder and zigzag wire. All three structures are taken in x-y plane and the wire is repeated in z- direction. After analyzing all the three isomeric structures, the linear wire configuration possesses minimum energy. The binding energy is calculated to be 3.24 eV/atom, which reflects strong bonding in comparison to other ladder and zigzag structures. They have binding energy equal to 3.23 and 3.16 eV/atom respectively. The value of total energy, internal energy and band energy is also minimum for linear structure. Next we consider the equilateral triangle for three atoms per unit cell. The atoms are taken in x-y plane and the triangle is repeated along the z-direction. The binding energy is calculated to be 3.36 eV/atom. In case four atoms we have considered four types of isomeric structures namely dumbbell, pyramidal, square and rhombus. The unit cell is again repeated in the z-direction. Among all the four structures we find that dumbbell structure possess highest binding energy i.e. 3.49 eV/atom and therefore exhibiting strong bonding structure. The total energy, internal energy, band energy is also minimum. For the five atoms per unit cell, we consider three types of structure namely pyramidal, tetrahedral and pentagonal. Here we predict that tetrahedral structure is the most stable ones having binding energy equal to 3.58 eV/atom. Since the other two structures have low BE and therefore treated to be unstable. For the five atom tetrahedral structure, four atoms lie in the x-y plane in the square form and one lies above the center of the square in the z-direction. The BE of pentagonal and pyramidal structure is 3.26 eV/atom and 3.50 eV/atom respectively. After extensive analysis all the calculated energies are found to be minimum for only tetrahedral structure which gives strong evidence for its stability. In order to explore the effect of hydrogen adsorption on Mg nanowire we have considered the most stable structure as predicted by us. The variation of energy with density of states (DOS) for all nanowires have been given in Figure 1. The highest peak occurs at -2.5 eV for most stabilized five atoms tetrahedral wire .

CONCLUSIONS :

The present ab-initio study of Mg nanowires Mg_n (n=1-5) reveals that all the wires are metallic in nature. We explore the lowest energy configuration and analyze stability and size effect on the electronic properties of different isomeric structures. The calculation of binding energy, the density of states (DOS) have been carried out in large energy interval. In the study of Mg nanowire, the binding energy of five atom tetrahedral wire is found to be highest and hence more stable. We find increase in B.E. with number of atoms. The total energy as well as band energy also varies. The maximum DOS is seen for five atom tetrahedral Mg nanowire. We predict that higher the DOS, higher the stability. The electronic structure study reveals the fact that it exhibits metallic character and sufficient number of channels is available for conduction and hence ballistic conductance is possible.

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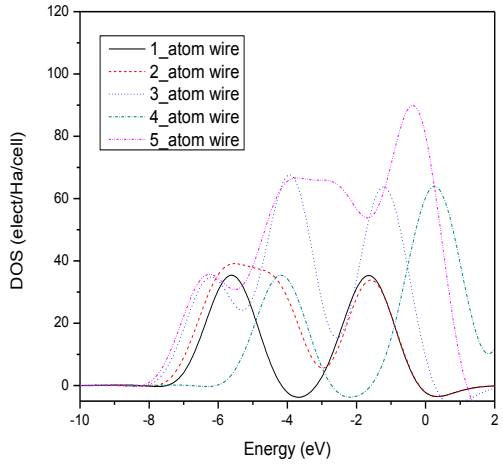

Figure-1. The variation of energy (eV) with density of states (DOS) for all nanowires.

Table-1. Isomeric structure of Magnesium nanowires containing one to five atoms per unit cell.The most stable structures are bold- faced ones.

Mg atoms per unit cell	Structure	Total energy (eV) per atom	Binding energy (eV) per atom	Internal energy (eV)	Band energy (eV)
one	**Linear**	**-31.47**	**3.16**	**-31.53**	**-11.63**
Two	**Linear**	**-31.55**	**3.24**	**-63.36**	**-21.28**
	Ladder	-31.54	3.23	-63.34	-21.26
	Zigzag	-31.46	3.16	-63.07	-20.75
Three	**Triangle**	**-31.66**	**3.36**	**-95.30**	**-29.40**
Four	**Dumbbell**	**-31.80**	**3.49**	**-128.60**	**-46.17**
	Pyramidal	-31.78	3.48	-127.56	-34.80
	Square	-31.74	3.44	-126.94	-35.00
	Rhombus	-31.74	3.44	-127.05	-35.09
Five	Pyramidal	-31.80	3.50	-158.33	-69.47
	Tetrahedral	**-31.88**	**3.58**	**-159.47**	**-86.91**
	Pentagonal	-31.56	3.26	-157.21	-41.17

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