Nanocomposites and nanomaterials

Durability of dichalcogenide MoS_2 nanoparticles with hydrogen intercalation

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Based on the method of pseudopotentials developed a model that allows us with the help of pair interatomic potentials to calculate the energy of interaction between the atomic layers of 2H-MoS2 intercalated with hydrogen and establish the probable location of intercalated hydrogen. The paper deals with the uniaxial deformation of materials. With the addition of the hydrogen atoms the unit cell volume also increases. Deformation is reduced to a change in one of the hexagonal lattice parameters (second one remains constant). The following model is proposed to solve this problem.

1. In the unit cell are added n_H hydrogen atoms. Calculate the total energy of the electron - ion system, provided that the parameter of basal planes remains unchanged, while the parameter c is changing.

2. At a minimum energy is determined the value of the crystal volume $\Omega(n_H)$ for each of n_H number of hydrogen atoms intercalated in a cell. The next step - a calculation of the interlayer interaction energy for each value of $\Omega(n_H)$.

The addition of hydrogen atoms does not change the energy of the interaction or the distance between the atomic layers of Mo - S. This means that the hydrogen atoms may not enter in the interlayer space Mo - S because of the strong interaction between them.

Was determined the functional dependence of the theoretical strength under uniaxial deformations σ_z on the amount of hydrogen in the direction c.

The hydrogen atoms intercalate between S - S atomic layers, while gradually increasing the distance between lattice planes and the theoretical strength decreases. With a further increase in the number of hydrogen atoms nH > 4 the energy of interaction of atomic layers tends to zero, the structure becomes thermodynamically unstable. Increasing of the thermodynamic instability is due to the fact that there is a concentration-dependent structural transition in dichalcogenides.