Heat conductivity process modelling in one-dimensional atomic chains

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Abstract

The problem of heat conductivity mechanisms of one-dimensional atomic 'non-metal' chains is considered. Heat conductivity concepts are evaluated. Simulation results for harmonic and non-harmonic atomic interactions are presented. The solitary waves mechanisms of heat conductivity realization is analyzed especially.

Keywords: one-dimensional atomic 'non-metal' chains, harmonic and non-harmonic atomic interactions, heat conductivity efficiency

1 Introduction

R Peierls was the first who paid attention to explanation of the thermal conductivity [1] (1929) .He have used Boltzmann concepts that had been developed by for the gas dynamics to phonons. HAowever, phonons cannot be localised with definite velocity, as can the molecules in a classical gas in accordance original Boltzmann equation.

F J Dyson has considered a chain of N masses [2] (1953), each coupled to its nearest neighbours by elastic springs obeying ***Hooke's law***. The longitudinal vibrations of the chain, all motions being supposed to take place in one dimension so that each mass is described by a single coordinate. The chain had mass m_j, and its displacement from its equilibrium position be x_j. The elastic modulus of the spring between particles j and $j+1$ be K_i. Then the equations of motion of the system are $m_j \ddot{x}_j = K_j(x_{j+1} - x_j) + K_{j-1}(x_{j-1} - x_j)$.

A Jackson and A D Mistriotis [3] have developed the lattice consisted of two types of particles with different masses. The odd-numbered particles have mass m_1, and the even-numbered have mass m_2. They interact with their nearest neighbours with an exponential force.

We pay attention to 'non-metal' one-dimensional atomic chains. However, for understanding the of the heat conductivity efficiency it is necessary to simulate to relative characteristic time of establishing of new phonon distribution state after external heat impact on the model atomic system. We consider various elastic atomic interactions (*Hooke's and non Hooke's type*) [4]. Moreover, non-Hooke interaction (e.g., exponential) leads to solitary wave mechanism of heat conductivity.

2 Conclusion

The harmonic waves mechanism for one-dimensional atomic 'non-metal' chains looks very limited for the most of physical cases and evidently wrong. The solitary waves mehanisms of heat condutivity is probably more reliable for it takes into account all possible and reasonable non-linear (non-harmonic) interatomic interactions.

References

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