

Nonlinear Gap Modes in a 1D Alternating Bond Monatomic Lattice with Anharmonicity

PAN Liu-Xian,^{1,2} ZHOU Guang-Hui,¹ XIA Qing-Lin³ and YAN Jia-Ren¹

¹ Department of Physics and Institute of Nonlinear Physics, Hunan Normal University, Changsha 410081, China

² Department of Physics, Yiyang Teacher's College, Yiyang 413049, Hunan Province, China

³ Department of Applied Physics, China Center South University, Changsha 410083, China

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Abstract: We analytically study the nonlinear localized gap modes in a one-dimensional atomic chain with uniform atomic mass but two periodically alternating force constants between the nearest neighbors by means of a quasi-continuum approximation. This model simulates a row of atoms in the <111> direction of a diamond-structure type of crystals or molecular crystals with alternating double and single bonds. For this lattice system, we find that the harmonic plus quartic anharmonic terms of inter-site potential produce a new type of nonlinear localized gap modes with a slightly asymmetry distribution of atomic displacements. These localized gap modes are somewhat different from widely studied localized gap modes with a symmetry atomic displacement distribution in diatomic ion lattices.

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Key words: diamond-structure lattice, nonlinear gap modes, quasi-continuum approximation

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