6
OTHER RESEARCH ACTIVITIES

The Computational Industrial Mechanics Programme continued the development of higher order "Nonlocal General Gradient Theory (NGGT)" for analyzing the nanoscale structures with two length scale parameters. We have determined the two length scale parameters by matching with atomic based lattice dynamics model. The present nonlocal general gradient theory has been investigated for one-dimensional dispersion in comparison with Peridynamic theory of micro structures. It has been observed that the Peridynamics model is in highly dispersive nature. The molecular dynamics simulation studies of nanotube/graphene structure have been extended to penta-graphene structure.

The new algorithm to extract spatio-temporal oscillations from noisy data developed at CSIR-4PI, extracts the multiple spatio-temporal components hidden in a synthetic noisy data typical of complex dynamical system. This algorithm will potentially lead to discovery of features that may provide radical insights in many branches of scientific research.

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6.1 Continuum and molecular simulations of Penta-Graphene

The superior mechanical properties of penta-graphene over graphene attracted the researchers to investigate this material. Unlike graphene, the penta-graphene behaves differently when subject to different mechanical loadings. Synthesis of penta-graphene is challenging work to researchers. The experimental set up at nanoscale is huge challenging task. So molecular dynamics investigations about penta-graphene behavior are initiated. Continuum modelling of penta-graphene with nonlocal models are also investigated.

6.2 Nonlocal General Gradient Theory for Nanostructures

The Eringen's nonlocal continuum models predicted the dispersion curves in better manner compared with classical continuum models. This model involves with one length scale parameter, which is in terms of internal characteristic scale like atom bond-bond length. Few higher order stress gradient models like Alavinasab model, Eringen second order models are predicted the dispersion of nanomaterials with one length scale parameter. The General Nonlocal Theory predicted the dispersion with two length scale parameters without matching the atomic model. The atomic model was used as benchmark to compare all these models. The Nonlocal General Gradient Theory model has been proposed with two-lengthscale parameters based on stress gradient approach. The bi-Helmholtz model can be obtained as special case from presently proposed model. Similarly other models are obtained from Nonlocal General Gradient Theory as special case. The terahertz frequencies are determined from Nonlocal General Gradient Theory and other models. From the Figure 6.1, it is very clear that the present proposed Nonlocal General Gradient model has predicted very good frequency results compared with other stress gradient

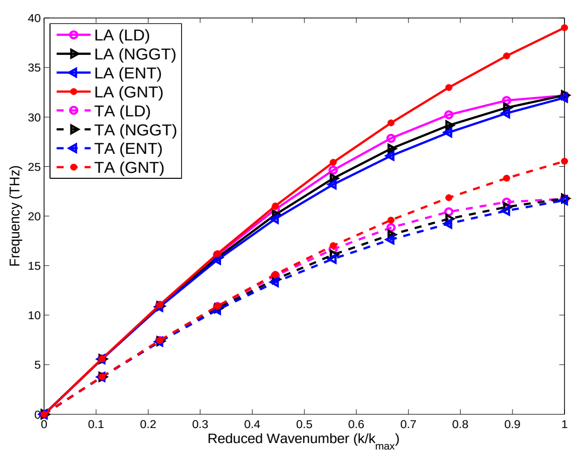

Figure 6.1 The dispersion characteristics of gradient models for Gr with Lattice Dynamics (LD), Nonlocal General Gradient Theory (NGGT), Eringen Nonlocal Theory (ENT), General Nonlocal Theory (GNT), Longitudinal Acoustic (LA), Transversely Acoustic (TA)

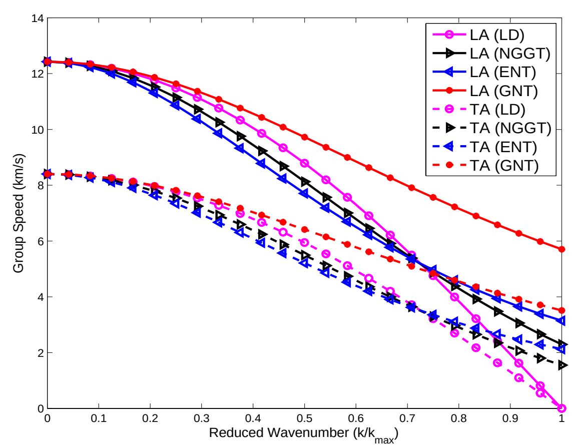

Figure 6.2 The group speed characteristics of gradient models for Gr with Lattice Dynamics (LD), Nonlocal General Gradient Theory (NGGT), Eringen Nonlocal Theory (ENT), General Nonlocal Theory (GNT), Longitudinal Acoustic (LA), Transversely Acoustic (TA)

models. The General Nonlocal Theory has been deviated and completely away in comparison with atomic results. Similarly the group speed has been obtained for all the stress gradient models along with Nonlocal General Gradient Model. Though the group speed (Figure 6.2) has been "badly off" in comparisons with atomic models, the present Nonlocal General Gradient Theory predicts better behavior than other stress gradient models.

6.3 Thermal wave dispersion of carbon nanorods with small-sized effects

The thermal effect on wave dispersion of carbon nanorod has been investigated using Eringen nonlocal continuum model. This phenomenon was not attempted in literatures due to certain modeling issues of thermal physics. The classical continuum fails to model the nanostructures because it does not associated with length scales. So the nonlocal continuum model with linear temperature change effect has been investigated in carbon nanorod. The low temperature and high temperature effects are considered in the present analysis. To represents the entire behavior of the system, the dimensionless parameters are used in the present study. To simulate the high temperature effect, the positive dimensionless parameters have been used. Similarly, the negative dimensionless parameters have been chosen for low temperature effects. At high temperature, the group speed increases with the increase of wave numbers up to certain "critical limit" and decreases with higher wave numbers (Figure 6.3). But the thermal effects are decreasing the nonlocal effects for increase in higher temperature effects. From the Figure 6.4, it has been observed that the wave numbers increases with the group speed at low temperature. Interestingly, the thermal effects are increasing with the "peak" and decreasing the nonlocal effects of carbon nanorod.

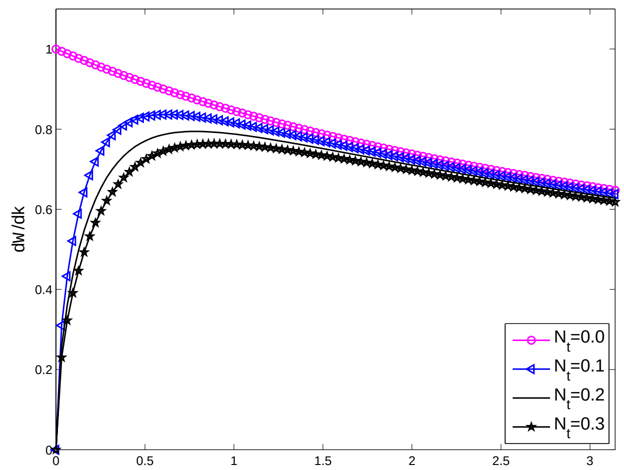

Figure 6.3 Thermal effect on carbon nanorod positive group speed

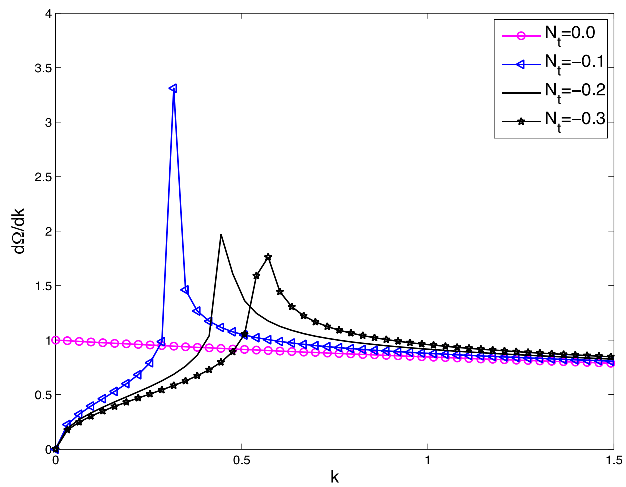

Figure 6.4 Thermal effect on carbon nanorod negative group speed

6.4 Nonlocal general gradient theory vs Peridynamics theory

Recently developed nonlocal general gradient theory for 1D bar has been investigated. This model consists of two different characteristics length scales. The Peridynamics model consists of one length scale parameter. Three different micromodulus (Case 1, Case 2 and Case 3) functions are considered in the present study. The Peridynamics models can be bond-based or state-based bar models. The Stress gradient nonlocal models proposed by Eringen, bi-Helmholtz model, Born-Karman, Alavinasab and Nonlocal General Gradient are compared with Peridynamics model. The dispersion curve and group velocity studies are carried out. Analytical expressions for group velocities are derived for the nonlocal models. The relation between the horizon and characteristic length are chosen to study the nonlocal Peridynamics and other nonlocal models. Further different nonlocal weight functions are used in the present wave characteristics studies. Among all the nonlocal models investigated in the present analysis, it has been found that the state based Peridynamics model is in highly dispersive nature.

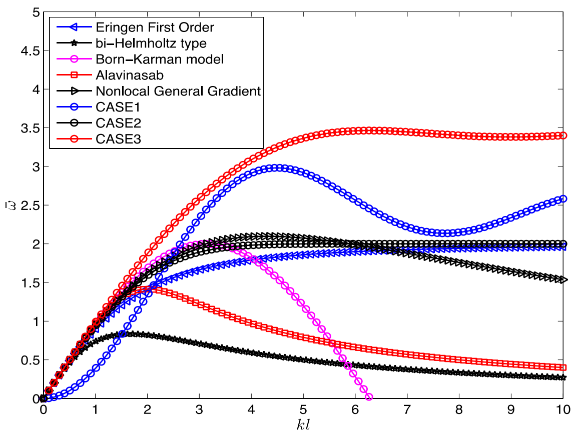

Figure 6.5 Dispersion of non-local models

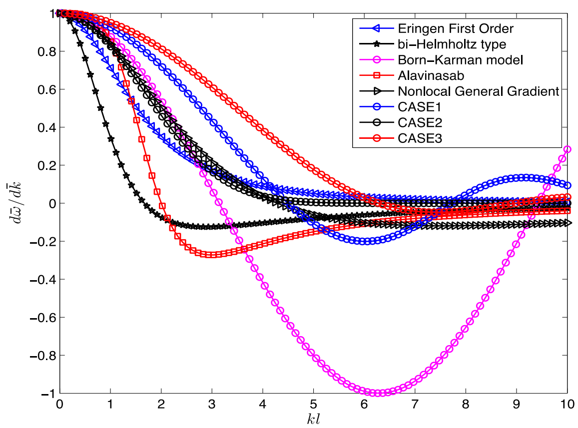

Figure 6.6 Group Velocity of non-local models

6.5 Decorated granular layers for impact decimation

We present dynamical simulations and simple mechanics arguments to propose a system of stacked blocks of square lattices of elastic spheres that can be used to decimate an incident impulse. Mass mismatch between adjacent blocks is accomplished by making the sphere radius in the upper block twice that of the lower block. The system decimates impact energies by converting the initial impulse into two solitary waves and then progressively into many smaller amplitude solitary waves. We also show that near perfect impact decimation capability can be realized with increased mass mismatch between adjacent blocks by creating sandwiched structures in which a block with smaller density spheres is surrounded on both sides with blocks of denser spheres. The proposed systems are expected to be scalable down to spheres of~100 nm and work for solid and hollow spheres.

6.6 An algorithm to extract spatio-temporal oscillations from noisy data

Spatio-temporal (ST) oscillations are fundamental to many natural and artificial systems. For a reliable numerical modeling and prediction of key signals pertaining to a dynamical system, it is essential to separate these ST signals, with least distortions, from a set of measurements. A common practice, in this context, is to extract the harmonic modes corresponding to significant peaks in a power spectral density. However, these significant peaks need not imply the existence of corresponding harmonic modes, if the temporal waveforms of one or more fundamental signals are not sinusoidal. Moreover, though the temporal periods of signals extracted by many modern linear decomposition methods (both uni- and multi-variate ones) are likely to be reliable, the corresponding spatial and temporal waveforms are not. In addition, the presence of noise in data makes the extraction even more unreliable. To address this serious limitation in the existing methodologies, a robust algorithm had been conceived and implemented based on a completely different criterion than those used in a Local Filter (*e.g.* Empirical Mode Decomposition) and in a Global Filter (*e.g.* Fourier Transform). It is necessary to recall here that the output from a Local Filter at a particular instance depends only on the characteristics within a time-window of fixed length chosen a priori. On other hand, outputs from Global Filter at given time have weighted influences, estimated by the minimization of a suitable loss function, from the variability at all other times. The new algorithm realistically extracts the multiple ST components hidden in a synthetic noisy data typical of complex dynamical system. The same strategy can also be employed to extract quasi-periodic ST signals. Hence, the proposed algorithm will potentially lead to discovery of features that may provide radical insights in many branches of scientific research.