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On energy balance and the structure of radiated waves in kinetics of crystalline defects

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ABSTRACT

Traveling waves, with well-known closed form expressions, in the context of the defects kinetics in crystals are excavated further with respect to their inherent structure of oscillatory components. These are associated with, so called, Frenkel–Kontorova model with a piecewise quadratic substrate potential, corresponding to the symmetric as well as asymmetric energy wells of the substrate, displacive phase transitions in bistable chains, and brittle fracture in triangular lattice strips under mode III conditions. The paper demonstrates that the power expended theorem holds so that the sum of rate of working and the rate of total energy flux into a control strip moving steadily with the defect equals the rate of energy sinking into the defect, in the sense of N.F. Mott. In the conservative case of the Frenkel–Kontorova model with asymmetric energy wells, this leads to an alternative expression for the mobility in terms of the energy flux through radiated lattice waves. An application of the same to the case of martensitic phase boundary and a crack, propagating uniformly in bistable chains and triangular lattice strips, respectively, is also provided and the energy release is expressed in terms of the radiated energy flux directly. The equivalence between the well-known expressions and their alternative is established via an elementary identity, which is stated and proved in the paper as the zero lemma. An intimate connection between the three distinct types of defects is, thus, revealed in the framework of energy balance, via a structural similarity between the corresponding variants of the 'zero' lemma containing the information about radiated energy flux. An extension to the dissipative models, in the presence of linear viscous damping, is detailed and analog of the zero lemma is proved. The analysis is relevant to the dynamics of dislocations, brittle cracks, and martensitic phase boundaries, besides possible applications to analogous physical contexts which are marked by macroscopic energy release through emission of waves and possibly linear viscous damping.

1. Introduction

The Frenkel–Kontorova model (Prandtl, 1928; Dehlinger, 1929; Frenkel and Kontorova, 1938) is a well-known paradigm in physics and mechanics that captures the essence of a large, and diverse, set of nonlinear phenomena (Braun and Kivshar, 2004). For example, it appears, directly or indirectly, in the context of mechanics of dislocations (Frenkel and Kontorova, 1938; Frank and Van der Merwe, 1950), martensitic phase boundaries (Abeyaratne and Vedantam, 2003; Slepyan et al., 2005; Truskinovsky and Vainchtein, 2005), cracks (Marder and Gross, 1995; Slepyan, 2002; Truskinovsky, 1996), friction at

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small scale (Tomlinson, 1929; Weiss and Elmer, 1997), absorbed monolayers (Braun and Kivshar, 2004), etc. Atkinson and Cabrera (1965) obtained an explicit solution for the steady-state problem of dislocation motion using the Frenkel–Kontorova model after introducing a simplification, with far-reaching consequences, that replaced the, original, sinusoidal substrate potential of Frenkel and Kontorova (1938) by a piecewise parabolic one. Further analyses and applications of the *simplified* Frenkel–Kontorova model, or its variants involving such snapping bond model, have appeared in several researches related to the mechanics of crystalline defects (including some classical works, for example, Weiner, 1964; Ishioka, 1973; Slepyan and Troyankina, 1984). A distinguishing feature of these simplified models, for prototype defect kinetics in crystals, is that the energy release, i.e. the expense of work by the driving force, involves the emission of *lattice waves* (also addressed as phonons, Kosevich, 2005; Celli and Flytzanis, 1970; Ishioka, 1971; Al'shitz and Indenbom, 1975; Marder and Gross, 1995; Carpio and Bonilla, 2003; Jin et al., 2008; Atrash et al., 2011), which allows an intuitive interpretation in the form of *macroscopic dissipation* (Slepyan, 2002). The associated notion of radiative damping has been well studied in different kinds of lattice models (Earmme and Weiner, 1977; Slepyan, 2001; Slepyan et al., 2005; Slepyan and Troyankina, 1984).

In the context of this paper, it is important to note that the expression for the kinetic relation (Truskinovsky, 1987; Abeyaratne and Knowles, 1991) (also known as friction law, mobility, etc.) for the case of asymmetric wells in Frenkel–Kontorova model, displacive phase transitions in bistable chains (Slepyan et al., 2005; Trofimov and Vainchtein, 2010), and brittle fracture (Marder and Gross, 1995; Kresse and Truskinovsky, 2004; Slepyan, 1981, 2002) is provided in terms of the real zeros of the dispersion relation ahead and behind the moving defect. Several distinguished researchers, and authors of several other related works, who study appropriate generalizations of the Frenkel–Kontorova model (or similar bistable chain models), have unambiguously established that the lattice mobility depends on the wave numbers of the radiated lattice waves. In the study of brittle fracture, using the two dimensional lattice models with piecewise linear interaction between particles, Slepyan (2010b, Section 2.3) (see also Slepyan, 2010a, 2002) established that the expression for the energy release can be also recovered from the balance of mechanical energy after accounting for the energy radiated through lattice waves. In this paper, an equivalent derivation of the kinetic relation is provided for the case of Frenkel–Kontorova model with unequal moduli using the elementary notions of the rate of working and the energy flux across a 'control volume' (strip). Moreover, the resulting expression is shown to be equivalent to that presented earlier. Analog of the same for the displacive phase transitions in bistable chains (Slepyan et al., 2005; Trofimov and Vainchtein, 2010) as well as the brittle fracture of triangular lattice strips (Marder and Gross, 1995) is also provided. Mott's idea of the energy balance (Mott, 1948; Dulaney and Brace, 1960; Ravi-Chandar, 2004; Freund, 1990; Hauch and Marder, 1998), during rapid crack growth, contains the relevant physical intuition. A microscopic version of Mott's energy balance has been applied, specially in the brittle fracture of triangular lattice strips. While staying in the physical domain, the average rate of working on a control strip and the supply rate of the total energy into the control strip is calculated directly in the paper. From the perspective of the radiated energy flux, it is found that the wave mode with lowest wavenumber, behind the crack tip, contributes substantially in the velocity regime where the traveling wave ansatz is known to be valid (Marder and Gross, 1995). The energy radiated per unit energy spent in bond snapping is graphically illustrated where the contribution of the *dominant wave mode* is also highlighted. The signature of quasi-one dimensional nature of the brittle fracture in lattice strips is thus affirmed (Marder and Gross, 1995). Using the alternate expression for the kinetic relation provided in this paper, the limiting case of the equal moduli for the case of Frenkel–Kontorova model, i.e. the dislocation mobility (Atkinson and Cabrera, 1965), is also obtained as a straightforward application of the analysis for the unequal moduli. Last but not the least, the energy balance admits an extension to the lattice models in the presence of (linear) viscous damping. The corresponding generalization of the conservative Frenkel–Kontorova model with unequal moduli (Marder and Gross, 1995; Kresse and Truskinovsky, 2004) is also studied and the special case of equal moduli (Kresse and Truskinovsky, 2007) is presented. A graphical illustration of the effect of such environmental viscosity is also provided. The application of these results to an analogous dissipative model of the displacive phase transitions in bistable chains and the brittle fracture in triangular lattice strip follows, in a manner similar to the conservative case, hence the details are omitted. The results established in this paper also find relevance in a forthcoming series of papers on dislocation kinetics. In general, the analysis draws upon the techniques and notational devices created by the author in a series papers on scattering of lattice waves by a crack in triangular lattice (Sharma, 2016a,b), as well as wave propagation in triangular lattice strips (Sharma, 2016c,e). In keeping with this, the derivations presented in this paper follow the notation applied therein. The paper brings the three distinct defects, i.e. phase boundary, dislocation, and crack, under the same framework via the zero lemma which is named after its analog in scattering theory (Sharma, 2016d).

1.1. Outline

In the first section of this paper, the concept of the mechanical energy balance in elastodynamics is briefly recalled. The traveling wave solution for Frenkel–Kontorova model with substrate potential incorporating asymmetric energy wells is recapitulated in the second section. The application of Wiener–Hopf technique, to obtain the exact expression for the traveling wave solution, is also briefly reviewed. The principle of the balance of mechanical energy on a moving control strip is shown to lead to an alternative expression for the energy release rate. The equivalence between the result based on radiated lattice waves and the well-known expression based on snapping bond criterion is established via the zero lemma. The same arguments of the energy balance are provided in the third section for the case of displacive phase transition in bistable chains and mode III brittle fracture of triangular lattice strips; the exact expression for the energy release rate and