International Journal of Engineering Science 128 (2018) 165–186

Contents lists available at ScienceDirect

International Journal of Engineering Science

journal homepage: www.elsevier.com/locate/ijengsci

Static and dynamic multipolar field expansions of dislocations and cracks in solids

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ARTICLE INFO

Article history:
Received 31 January 2018
Revised 13 March 2018
Accepted 15 March 2018

Keywords:
Dislocations
Cracks
Elastodynamics
Multipole field
Dipole moments

ABSTRACT

This article provides a comprehensive analysis of the way multipolar field expansions, of common use in the study of point defects in solids, may be extended to study the long range fields of dislocations and cracks. The long range fields of such defects are of relevance in fields as disparate as dislocation dynamics, microcrack and fragmentation, or radiation damage studies. The article provides a general framework for the development of multipolar field expansions in the continuum; one that may be used for any generalised force distribution. The general framework is combined with the Burridge–Knopoff force representation of dislocations and cracks, both in the planar and in the three dimensional cases, to achieve their respective multipolar field expansions for generalised dislocation loop and crack geometries. It is shown that, despite its simplicity, the multipolar field expansions provide a very accurate measure of the far field of both planar and three dimensional dislocations and cracks, and that the accuracy increases as higher order terms (i.e., quadrupolar, octopolar, etc) are introduced into the expansion. The formulation is then extended to the elastodynamic case. Both a spatial-temporal multipolar field expansion and a spatial multipolar field expansion, are developed. The spatial-temporal multipolar field expansion is seen to capture only the leading terms of the elastodynamic fields, whilst the spatial multipolar expansions are seen to be very accurate at capturing the long range field behaviour so long as the characteristic speed of the dislocation or crack are a fraction of the longitudinal speed of sound.

1. Introduction

This article concerns the multipolar field expansions of the elastic fields of dislocations and cracks. By the *multipolar expansion of an elastic field* we mean the approximation of that same elastic field as a set of force multipoles which are applied over a single point, their distributional complexity increasing with the expansion's order, and their magnitude dependent on the actual field's underlying characteristics. Thus, an otherwise arbitrary and extended elastic field, as would be that of a dislocation loop or a three dimensional crack, may be approximated as a set of point force dipoles, quadrupoles, octopoles, etc, applied on a single point. The result of the expansion is meant to be an approximation that captures correctly the energetics and the long range behaviour of the elastic field, even if the near field is incorrectly approximated. Because it is the result of the application of simple point forces of constant albeit well-defined magnitude, the multipolar expansion will generally be simpler to evaluate than the original elastic field.

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https://doi.org/10.1016/j.ijengsci.2018.03.012

Multipolar expansions of this sort were originally developed in electrodynamics, for the study of long range electromagnetic fields of charge distributions (Jackson, 1999): by approximating the long range potential as if they originated on a multipole of point charges, one can greatly simplify the study of the distribution's long range effects. This has proven to be a fruitful avenue of research, particularly in the study of the electronic structure of complex molecules (Ojeda-May & Garcia, 2010), and in spectroscopy (Yurkin & Hoekstra, 2007), amongst many other examples.

One of the classical results derived from the study of crystal defects in elastic solids is that of the force multipole models of point defects. As in the electrodynamic case, this is aimed at producing an elastic model of the point defect as a set of forces (see for instance Balluffi, 2017; Teodosiu, 1982), and at being able to study their long range effects and interactions from an energetically consistent perspective. This article generalises this approach to the modelling of dislocations and cracks. This generalisation is based on one of the crucial results by Backus and Mulcahy (1976a,b), namely that the moment tensor and the force representations of an elastic source can be given in terms of their '*polynomial moments*'. In parallel, and within the context of non-linear elasticity, Kunin (1968) showed that the fields of arbitrary inhomogeneities may be expressed in terms of perturbations of the boundary conditions, that enabled expressing the fields of the defect as a series expansion reliant on the homogeneous, infinite medium's Green's function.

Traditionally, the use of multipolar expansions in the theory of dislocations was associated with the use of clusters of dislocations (e.g., dipoles, quadrupoles,… of edge or screw dislocations) as a way of computing their collective long range effects on other such clusters (Chen, Gilman, & Head, 1964; Hirsch, 1975; Wang & LeSar, 1995). In addition, based on Kunin's theory, Kosheleva and coworkers (Kosheleva, 1983; Vakulenko & Kosheleva, 1980) applied multipolar field expansions to the theory of composite media.

In recent years, a number of more sophisticated multipolar expansions related to the computation of dislocation interactions (LeSar & Rickman, 2002; Zhao, Huang, & Xiang, 2010) and the elastic fields of dislocations (Dudarev & Sutton, 2017; Wang, Ghoniem, & LeSar, 2004) have been offered in the context of extending the fast multipole technique (Greengard & Rokhlin, 1987) to dislocation dynamics simulations and dislocation theory; in this way, they offer a considerable speed up factor compared to conventional discrete dislocation dynamics methods, and enable more cost effective theoretical treatment of the long range interactions between dislocations and other crystalline defects (Dudarev & Sutton, 2017). As opposed to the full multipolar expansion offered in this article, these methods are based on the dipolar field expansion of the elastic energy (LeSar & Rickman, 2002; Zhao et al., 2010) and the stress tensor (Wang et al., 2004); they are, therefore, multipolar expansions of the moment tensors, based on De Wit's line integral formalism (De Wit, 1960). Furthermore, other formulations of multipolar field expansions have recently been employed to study the far field asymptotic field of the elastic fields generated by inhomogeneities (Sevostianov & Kachanov, 2011), and in the context of homogenisation theory (Kushch & Sevostianov, 2015).

This article generalises these efforts, and extends them to higher order multipolar moments, to elastic anisotropy, and to elastodynamics, offering a comprehensive theoretical framework with which to develop further multipolar expansions of extended defects, as we do for cracks in this work. In both the static and elastodynamic cases, we show that the multipolar field expansions correctly capture the long range behaviour of dislocations and cracks, to increasing accuracy as the multipolar moments' order is increased. As will be seen, by applying the representation theorem we make the multipolar expansion generally anisotropic, and dependent on Green's tensor function and the dislocation's or crack's moments of area. We argue that such expansions are of relevance to the study of either defect when their representative lengths are small compared with the scale of the problems. For dislocations, this could refer to the study of nano-loops resulting from radiation damage, or to the study of the collective behaviour of dislocations in an statistical manner. For cracks, the formulation we present would be of relevance to all those applications where microcracks are present, particularly if their numbers are large: from damage in semiconductors, to fragmentation studies, in all those cases small cracks will interact with one another not so much via their near fields but through their long range fields, and the multipolar field expansions we introduce in this article offer an exact and cost-effective description of these very long range effects.

The methodology introduced in this article relies on employing the dislocation's and crack's force representation, as opposed to their eigenstrain or eigenstress representations. The need for a force representation arises in Section 2, where we offer the multipolar field expansion of a general displacement field. We shall see that, in the same way the multipolar field expansions of point defects require their description as sets of forces, the true multipolar field expansion of any other extended defect requires it too. Thus, in Section 3 we provide the elastostatic force representation of both dislocations and cracks by means of the Burridge–Knopoff theorem (Burridge & Knopoff, 1964), which we briefly discuss. This formulation will provide the way of attaining higher order multipolar moments. Having defined the general expression of a multipolar field expansion and provided the force representation of a general dislocation loop, in Section 4 we develop the theory of multipolar expansions of loop. We show that in the most general case of a dislocation loop, the multipolar field expression depends to increasing orders on the moments of area enclosed by the loop, leading to a simple and cost-effective formulation of the long range effects of dislocations. In Section 6, we apply the very same formulation to cracks in a number of modes and geometries; albeit the number of cases considered here is non-exhaustive, we show the procedure to develop the multipolar field expansion of any one crack. In Section 7 we go on to extend the formulation to the case of elastodynamic, multipolar field expansions both for dislocations and cracks.