Bi-continuum modelling of layered structures and crystalline interfaces

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Summary: The bi-continuum model composed of two interpenetrating and dynamically coupled material continua is analysed as a simplified but relatively accurate way to describe some physical phenomena in crystalline solids. The essential novelty of our approach consists in treating a crystalline medium as a bi-continuum, even if the crystalline lattice is structurally single-component. Particular attention is paid to the oscillatory behaviour of solutions on the atomic level. Starting from a discrete atomic chain, the basic formulation of the bi-continuum model is derived. The essential features of the model, including accuracy of the results as functions of physical parameters, are discussed.

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1 Introduction

Discrete structural models such as atomic lattices or stratified structures are capable of delivering, as a rule, highly reliable and accurate results concerning a wide range of physical phenomena in solid matter. Most frequently, however, to produce such results, an atomic model has to be treated with the aid of computer simulation techniques, what imposes severe restrictions on the size of computed samples and leads to the lack of generality in the results. Moreover, atomic models are sensitive to details of the interatomic potentials; the final reliability of results depends critically on the reliability of the potentials used. In consequence, simplified models which may produce analytical—although less accurate—results are still highly desirable. The loss of accuracy should not, however, be catastrophic.

In the present paper we focus our attention on atomic configurations in complex layered structures or in the vicinity of planar or quasi-planar crystalline interfaces [4]. In such situations, the configurations frequently exhibit a sign-alternating behaviour [1, 3] on atomic scale, not reproducible by a simple classic continuum. We have found, however, that such a behaviour can be described by an appropriately chosen two-component continuum model, called the bi-continuum.

The concept of multi-continuum, understood as a material medium on which several displacement fields are defined, is intuitively evident when one considers multicomponent media (like e.g. mixture of substances with different physical properties or the medium composed of electrons considered as one component and heavy ions as the other one).

The idea given in [2] was to introduce the multicontinuum description for structurally complex media, even if such a medium has only one component. The different displacement fields are defined on different substructures. We shall show how the idea of multicontinuum works in the case when multi=2.

From the point of view of independent variables, the problem is essentially one-dimensional. The corresponding variable will be denoted by $x$ with, according to the needs, appropriate indices or diacritics. For the sake of simplicity, we perform our theoretical constructions on linear atomic chains, although in the real three-dimensional applications the ”atoms” are intended to represent whole crystalline planes or appropriate structural layers.

In Sections 2 and 3 we state the problem for a homogeneous atomic chain and examine the sign-alternating solutions near the ”interface”. In Section 4 we analyse a composite linear chain, consisting of two components. This provides the basis for construction of the bi-continuum model in Section 5. Subsequently we solve the interface problem in atomic and bi-continuum models, respectively, compare the solutions, and discuss the resulting degree of approximation.

2 Homogeneous atomic chain

Let us consider an atomic chain with interactions between the first and second nearest neighbours. Let $u_i$ denote the displacement of the atom number $i$ from its equilibrium position. By $\kappa_f, n_f$ and $\kappa_s, n_s$ we denote the elastic constant and initial stretch connected with shorter and longer bonds, respectively.
The energy of a short bond is given by the formula

\[ W_f = \frac{1}{2} \kappa_f (\nabla_1 u)^2 + n_f \nabla_1 u \]  

while that of a long one by

\[ W_s = \frac{1}{2} \kappa_s (\nabla_2 u)^2 + n_s \nabla_2 u, \]  

where \( \nabla_1 \) and \( \nabla_2 \) are symbols of the central difference operators acting on displacements of the first and second neighbours, respectively. The elastic energy of the chain equals the sum over all the bonds.

The state of equilibrium of a homogeneous chain is described by the set of equations

\[ \kappa_f (u_{i-1} - 2u_i + u_{i+1}) + \kappa_s (u_{i-2} - 2u_i + u_{i+2}) = 0, \]  

where the index \( i = 1, 2, 3, \ldots \). The general solution to equations (3) is given by the function

\[ u_i = Az^i + Bz^{-i} + Ei + C \]  

with arbitrary constants \( A, B, E, C \), and

\[ z = -\beta + \sqrt{\beta^2 - 1}, \]  

where

\[ \beta = \frac{\alpha}{2} + 1, \quad \alpha = \frac{\kappa_f}{\kappa_s}. \]  

3 Atomic chain with "interface"

Now, instead of a homogeneous chain we shall consider two semi–infinite homogeneous parts (of possibly different materials) connected by an ‘interface’ modelled by intermediate bonds of the third kind. The quantities related to the intermediate bonds will be labelled by the superscript \( o \), while the superscripts \( - \) and \( + \) will refer to the left and right semi–infinite chains, respectively.
For simplicity we assume that the parameter $\alpha$ has the same value for all three materials,

$$\frac{\kappa_f^+}{\kappa_s^+} = \frac{\kappa_f^0}{\kappa_s^0} = \frac{\kappa_f^-}{\kappa_s^-} = \alpha.$$  (7)

Moreover, we assume that

a) the homogeneous chains are in equilibrium,

b) there are no forces at infinity.

The above conditions imply the following relation between the initial stretch forces:

$$n_f + 2n_s = 0,$$  (8)

which means that the sum of forces transmitted by any section vanishes.

The solution of such an interface problem is given by

$$u_j = \begin{cases} 
\frac{\varepsilon_-}{1 - z} z^{-j-1} & \text{for } j = -1, -2, \ldots \\
A - \frac{\varepsilon_+}{1 - z} z^{j-1} & \text{for } j = 1, 2, \ldots ,
\end{cases}$$  (9)

where $z$ is defined by the formula (5). Displacements are calculated relative to the asymptotic value at $-\infty$. The asymptotic value at $+\infty$ is given by

$$A = \varepsilon_o + \frac{\varepsilon_- + \varepsilon_+}{1 - z}.$$  (10)

The symbols $\varepsilon_-, \varepsilon_o$ and $\varepsilon_+$ denote deformations and are expressed by material parameters as follows:

$$\varepsilon_- = -T_1(\varepsilon_o + \frac{1}{\kappa_s^0}(n_s^o - n_s^-)),$$  (11)

$$\varepsilon_o = \frac{1}{\kappa_s^0}(2\beta - T_1 - T_2)^{-1}(T_1(n_s^o - n_s^-) - T_2(n_s^+ - n_s^o)),$$  (12)

$$\varepsilon_+ = T_2(\varepsilon_o - \frac{1}{\kappa_s^0}(n_s^+ - n_s^o)),$$  (13)

where we have introduced the auxiliary notations

$$T_1 = (1 - \frac{\kappa_s^-}{\kappa_s^0}(1 + \frac{1}{z}))^{-1},$$  (14)

$$T_2 = (1 - \frac{\kappa_s^+}{\kappa_s^0}(1 + \frac{1}{z}))^{-1}.$$  (15)

The resulting solution is represented by sharp-bend vertices of the line in Fig. 3.

Let us notice that the number $z$ is always negative. It implies a strongly oscillating character of the solution given by formula (9): the nearest neighbours are displaced in opposite directions. Thus every second atom is displaced in the same direction. Hence, as a result of the presence of the second neighbour interactions, we have obtained a polarization of the chain, expressed as a relative displacement of both substructures.
4 Composite atomic chain

To construct the bi-continuum model we start from introduction of two fields of displacements: \( v \) and \( w \), each of them defined on one of the sub-chains.

![Fig. 2. Heterogeneous atomic chain](image)

We shall describe by the indices \( x \) and \( \bar{x} \) the position of "black" and "white" atoms supporting the fields \( v \) and \( w \), respectively. The description may be applied to two-component structures as well as to one-component but dimerized ones. Altogether, in the translationally invariant case we have four classes of bonds. Two bonds between the first neighbours are characterised by parameters \( \kappa_f, n_f \) and \( \bar{\kappa}_f, \bar{n}_f \), while two other bonds, between the second neighbours, are characterised by \( \kappa_s, n_s \) and \( \bar{\kappa}_s, \bar{n}_s \). If there are no forces at infinity, then the sum of forces transmitted by any section vanishes,

\[
\begin{align*}
n_s + n_f + \bar{n}_s &= 0, \\
n_s + \bar{n}_f + \bar{n}_s &= 0.
\end{align*}
\]

This fact implies, in turn, that initial stretches of bonds between the nearest neighbours equal each other:

\[
n_f = \bar{n}_f.
\]

The symbol \( a \) denotes now the distance between the closest atoms of the same colour (which corresponds to \( 2a \) in the previous sections), \( b \) and \( c \) denote the distances between atoms of different colours. These quantities are connected by the relation

\[
b + c = a.
\]

The energy of the chain can be composed of 4 parts, each one connected with one kind of bonds,

\[
W = W_s + \bar{W}_s + W_f + \bar{W}_f,
\]

where

\[
\begin{align*}
W_s &= \sum \left( \frac{1}{2} \kappa_s (v_x - v_{x-a})^2 + n_s (v_x - v_{x-a}) \right), \\
\bar{W}_s &= \sum \left( \frac{1}{2} \bar{\kappa}_s (w_\bar{x} - w_{\bar{x}+a})^2 + \bar{n}_s (w_\bar{x} - w_{\bar{x}+a}) \right),
\end{align*}
\]
\[ W_f = \sum \left( \frac{1}{2} \kappa_f (v_x - w_x)^2 + n_f (v_x - w_x) \right), \]
\[ W_{\bar{f}} = \sum \left( \frac{1}{2} \bar{\kappa}_f (w_{\bar{x}} - v_{\bar{x} - a})^2 + \bar{n}_f (w_{\bar{x}} - v_{\bar{x} - a}) \right). \] (20)

The last two parts of the energy contain terms combining values of different fields at different points. We shall express these terms with the help of fields \( \bar{v} \) and \( \bar{w} \) which interpolate the fields \( v \) and \( w \) to the whole chain. By definition,
\[ \bar{v}_x = \frac{\kappa_f v_x + \bar{\kappa}_f v_{x-a}}{\kappa_f + \bar{\kappa}_f}, \quad \bar{v}_x = v_x \] (21)
and
\[ \bar{w}_x = \frac{\bar{\kappa}_f w_{x+a} + \kappa_f w_x}{\kappa_f + \bar{\kappa}_f}, \quad \bar{w}_x = w_x. \] (22)

Using these interpolating fields, we can express the energy of the first neighbour bonds by
\[ W_f = \sum \left( \frac{1}{2} \kappa_f [(v_x - \bar{w}_x) + \frac{\bar{\kappa}_f}{\kappa_f + \bar{\kappa}_f} (w_{x+a} - w_x)]^2 + n_f [(v_x - \bar{v}_x) + \frac{\bar{\kappa}_f}{\kappa_f + \bar{\kappa}_f} (w_{x+a} - w_x)] \right), \] (23)
\[ W_{\bar{f}} = \sum \left( \frac{1}{2} \kappa_f [(w_x - \bar{v}_x) + \frac{\kappa_f}{\kappa_f + \bar{\kappa}_f} (v_x - v_{x-a})]^2 + \bar{n}_f [(w_x - \bar{v}_x) + \frac{\kappa_f}{\kappa_f + \bar{\kappa}_f} (v_x - v_{x-a})] \right). \] (24)

All the differences are now expressed either by two fields at the same point, or by one field at different points.

5 The bi-continuum

We arrive at the corresponding bi-continuum expression for energy by appropriate truncations of the Taylor series. As the simplest possibility let us consider the correspondence
\[ (1) \quad \nabla f \longrightarrow a f', \]
\[ (2) \quad \sum \longrightarrow \frac{1}{a} \int, \]
\[ (3) \quad \bar{f} \longrightarrow f. \] (25)

The symbol \( f \) represents here an arbitrary function, the dash denotes the derivative with respect to \( x \), and \( a \) – the lattice parameter. The set of rules (25) will be referred to as the correspondence of order 0. We shall consider also another set of rules, called correspondence of order 1, which takes into account the microstructure of the elementary cell of our composite chain. Namely, instead of rule (3) in (25), we take
\[ (3a) \quad \bar{v} \longrightarrow v + \frac{\bar{\kappa}}{\kappa_f + \bar{\kappa}_f} v', \]
\[ (3b) \quad \bar{w} \longrightarrow w - \frac{\bar{\kappa}}{\kappa_f + \bar{\kappa}_f} w', \] (26)
where
\[ \bar{\kappa} = \kappa_f c - \bar{\kappa}_f b. \] (27)
If $\tilde{\kappa}_f = \kappa_f$ and $b = c$, then both the correspondence rules are equivalent. Let us note that the transition to correspondence rules of order 1 does not augment the order of equations.

Using the correspondence rule of order 0 one obtains the following formulae for energies of the corresponding bonds:

$$W_s = \int \left( \frac{a}{2} \kappa_s v'^2 + n_s v' \right) dx,$$
(28)

$$W_\tilde{s} = \int \left( \frac{a}{2} \bar{\kappa}_s w'^2 + \bar{n}_f w' \right) dx,$$
(29)

$$W_f = \frac{1}{2a} \int [\kappa_f (v - w + \frac{\bar{\kappa}_f}{\kappa_f + \bar{\kappa}_f} aw')]^2 + an_f (v - w + \frac{\bar{\kappa}_f}{\kappa_f + \bar{\kappa}_f} aw')] dx,$$
(30)

$$W_\tilde{f} = \frac{1}{2a} \int [\bar{\kappa}_f (w - v + \frac{\kappa_f}{\kappa_f + \bar{\kappa}_f} av')]^2 + an_f (w - v + \frac{\kappa_f}{\kappa_f + \bar{\kappa}_f} av')] dx.$$
(31)

In the last expression the equality (17) has been used. The energy connected with the n.n. bonds may be rewritten in the form

$$W_f + W_\tilde{f} = \frac{1}{2a} \int [(\kappa_f + \bar{\kappa}_f)(v - w)^2 + a^2 \frac{\kappa_f \bar{\kappa}_f}{(\kappa_f + \bar{\kappa}_f)^2} (\bar{\kappa}_fw'^2 + \kappa_f v'^2)$$
$$+ \frac{an_f}{\kappa_f + \bar{\kappa}_f}(\bar{\kappa}_fw' + \kappa_f v')] dx + \text{boundary term}.$$  
(32)

The correspondence rule of order 1 introduce definite corrections to the above formulae. These corrections result in

a) an additional coupling term of the form $(v - w)(v' + w')$,

b) renormalisation of coefficients in other terms.

In consequence, the energy density of the homogeneous bi-continuum takes the form

$$w_d = \frac{1}{2} ev'^2 + \frac{1}{2} gw'^2 + \bar{\kappa}(v - w)(v' + w') + \frac{1}{2} h(v - w)^2,$$
(33)

with the phenomenological coefficients. One can connect them with parameters of the discrete model by the following equalities:

$$e = a\kappa_s + a\bar{\kappa}_f \left( \frac{\kappa_f - \bar{\kappa}_f}{\kappa_f + \bar{\kappa}_f} \right)^2,$$

$$g = a\bar{\kappa}_s + a\kappa_f \left( \frac{\bar{\kappa}_f - \kappa_f}{\kappa_f + \bar{\kappa}_f} \right)^2,$$

$$h = \frac{\kappa_f + \bar{\kappa}_f}{a},$$
(34)

and $\bar{\kappa}$ is given by the formula (27).

The equations of static equilibrium for a homogeneous medium have the form

$$ev'' - 2\bar{\kappa}w' - h(v - w) = 0,$$

$$gw'' + 2\bar{\kappa}v' + h(v - w) = 0,$$
(35)
and, without forces at infinity, have the general solution

\[ v = \begin{cases} 
Ae^{-\zeta x} + C, & \text{for } x > 0, \\
Be^{\zeta x}, & \text{for } x < 0,
\end{cases} \]

\[ w = \begin{cases} 
Ak_1e^{-\zeta x} + C, & \text{for } x > 0, \\
Bk_2e^{\zeta x}, & \text{for } x < 0.
\end{cases} \]  \hspace{1cm} (36)

with the exponent coefficient expressed by material constants according to the formula

\[ \zeta^2 = \frac{h(e + g) - 4\bar{\kappa}^2}{eg}. \]  \hspace{1cm} (37)

The coefficients connecting amplitudes of fields \( v \) and \( w \) equal

\[ k_1 = \frac{h - \zeta^2 e}{h - 2\zeta \bar{\kappa}}, \quad k_2 = \frac{h - \zeta^2 e}{h + 2\zeta \bar{\kappa}}. \]  \hspace{1cm} (38)

In the case of exact inversion symmetry, when \( \kappa_s = \bar{\kappa}_s, b = c, \kappa_f = \bar{\kappa}_f \) and then \( \bar{\kappa} = 0 \),

\[ \zeta^2 = \frac{2h}{e}, \quad k_1 = k_2 = -1. \]  \hspace{1cm} (39)

In the next section we shall consider such a symmetric case.

6 Comparison between bi-continuum and discrete solutions

The solution of the bi-continuum interface problem may be constructed from functions (36), with appropriate values of constants \( A, B, C \). The simplest way to match this solution to its discrete counterpart is to request that values of corresponding branches of functions \( u, v \) and \( w \) coincide at the atoms nearest to the interface. Two such conditions plus coincidence of asymptotic values will be sufficient to calculate \( A, B \) and \( C \). In this way, making use of (12), we have

\[ C = \frac{T_1(n_s^0 - n_s^-)}{\kappa_s^0(\beta - T_1)}, \]  \hspace{1cm} (40)

and, for the other constants

\[ A = B = -\frac{\varepsilon_1}{1 - z} e^{\zeta a/4}. \]  \hspace{1cm} (41)
The bi-continuum fields $v$ and $w$ are plotted in Fig. 3.

![Fig.3. Exemplary discrete and bi-continuum solutions; $\alpha = 0.05$, $\kappa = 1.5$, $n = 1.5$]

The upper branches correspond to the field $w$. The values of discrete function $u$ correspond to the sharp-bends of the broken line.

![Fig.4. Error in s.n.n. displacement vs. $1/\alpha$]

To examine the accuracy of the bi-continuum model, the error in value of fields $v$ and $w$ at the distance $3a/4$ from the interface, equivalent to the second nearest neighbours, is plotted vs. $1/\alpha$ in Fig. 4. The error corresponding to $\alpha = 0.05$ equals about 4 percent of the lattice constant. Note that, under the assumed correspondence rules, the error does not
change the sign.

Another way to compare the atomic and bi-continuum models is to analyse the relation between the local dimerisation ranges or, equivalently, between the exponents in both models. Let us note that, since the symbol $a$ denotes the distance between the second n.n., one should calculate the discrete exponent $\lambda$ from the equation

$$z^2 = e^{-\lambda a}, \quad (42)$$

which, according to (5), implies the dependence of $\lambda$ on $\alpha$. On the other hand, for the bi-continuum model, by making use of equations (39) and (34), one obtains

$$\zeta^2 = \frac{16}{a^2} \frac{\alpha}{4 + \alpha}. \quad (43)$$

The above equation implies $0 < a\zeta < 4$.

![Graph](image.png)

**Fig. 5.** Local dimerisation range, $1/\lambda$ vs. $1/\zeta$

The dependence of $1/\lambda$ on $1/\zeta$, is plotted in Fig. 5 as the lower curve to be compared with the line $\lambda = \zeta$. A substantial difference is present only at distances smaller than the lattice constant $a$. 
To enable a more precise estimation of the error, the difference $1/\lambda - 1/\zeta$ is plotted vs. $1/\alpha$ in Fig. 6.

![Graph showing the difference between dimerisation ranges: $1/\lambda - 1/\zeta$ vs. $1/\alpha$.](image)

### 7 Final remarks

We have presented a method of construction of the bi-continuum model based on a heuristic system - a linear atomic chain. One may, however, forget about the derivation, and consider the obtained equations as phenomenological ones. Generally, it is not necessary to relate the phenomenological coefficients to the parameters of an atomic model. The fairly good agreement between the bi-continuum and atomistic solutions can be treated as an argument in behalf of our model, at least in the sense that we have not made gross errors.

The internal structure of the "atoms" in the chain may be complex – they need not be interpreted as material points. As an important example one can mention atomic planes of 3D crystalline structures, in particular the oxygen-copper planes, or even the octahedral layers in high temperature superconducting materials. If our "atoms" are planes or layers, one should replace, in the expression for energy, the scalar quantities by appropriate vectors and matrices. And the construction will run analogically, under the condition that one takes into account the interactions of the first and second n.n. between planes or layers. Similarly one can consider layered structures in the form of arrays of Josephson junctions. Such systems occur in a natural way in superconducting crystals, or else they can be shaped artificially in a technological way.

How important are the planar interfaces? There are many cases where they are important by themselves. It is expedient to notice that (what we call) the "planar" interfaces need not be strictly planar. It is sufficient that the curvatures of the corresponding surfaces should be not too high as compared with the characteristic exponents (both of dimension $cm^{-1}$, ...
The interfaces can also affect the bulk properties of materials. It concerns the materials which contain a lot of interface area per unit volume. Also this property can be expressed by a parameter of dimension of inverse length which is particularly high for nanostructured materials.

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