Active Free Surface Density Maps

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Abstract. Percolation problems were occupied to many physical problems after their establishment in 1957 by Broadbent and Hammersley. They can be used to solve complex systems such as bone remodeling. Volume fraction method was adopted to set some algorithms in the literature. However, different rate of osteoporosis could be observed for different micro-structures which have the same mass density, mechanical stimuli, hormonal stimuli and nutrition. Thus it was emphasized that the bone might have identical porosity with different specific surfaces. Active free surface density of bone refers the used total area for its effective free surface. The purpose of this manuscript is to consolidate a mathematical approach which can be called as “active free surface density maps” for different surface patterns and derive their formulations. Active free surface density ratios were calculated for different Archimedean lattice models according to Helmholtz free energy and they were compared with their site and bond percolation thresholds from the background studies to derive their potential probability for bone remodeling.

1. From Historical Bone Investigations to Novel Formulation
In 1957, Broadbent and Hammersley established the percolation theory to explain the random properties of the flow through a medium. After then the theory was used to solve many physical problems [1]. It may be a beneficial tool to investigate complex systems such as bone remodeling. In the literature, some equations were proposed which were based on volume fraction method [2, 3]. However, different osteoporosis rates were reported for different micro-structures which have the same environmental conditions. Thus it was emphasized that the bone had identical porosity although it had different specific surfaces [4-7]. “Mass and the mechanostat” concept was suggested to describe osteoblast and osteoclast tasks for the bone by Frost [8]. In fact, Wolff’s law was caused an awareness for the changeability of bone architecture according to the applied external stress in 1892 [9]. However, Frost, Cowin, Huiskes et al. reported that the strain value was important [8,10,11]. Huiskes et al. investigated the strain energy density (SED) to conduct mechanical signals for remodeling of the bone structure [11]. Skerry et al. proposed that the osteocyte should be a mechanosensor of bone [12]. It was reported that it delivered mechanical signals to activate osteoblasts and osteoclasts [12, 13]. Thus small-strain approach was developed [2-14]. The free surface density of bone was explained as the total surface area which was in contact with soft tissue (Figure 1) [4-7]. Martin reported the importance of specific surfaces of bone on osteoblast and osteoclast activity. His reports were culminated in a conclusion that the higher specific surface area, the greater bone remodeling potential. Thus the potential of bone remodeling should be related with morphology and dimensions of the specific surface [4-7].
Martin proposed an empirical formula for effective free surface density \[4-6\]. After then Rouhi et al. redeveloped it for elliptical and different hypothetical micro-structural geometries \[7\]. Their arguments need to be updated in several respects. There is a research gap for a novel theory which includes random networks between Archimedean lattice models for bone remodeling. The most important development should be “the description of a dispersion error factor”. In the present paper, I report my theoretical study as “Active Free Surface Density (AFSD) Maps” to derive a novel equation for bone remodeling. AFSD ratios were calculated for different Archimedean lattice models according to Helmholtz free energy and they were compared with their site and bond percolation thresholds from the background studies to derive their potential probability for bone remodeling.

2. Material and Method

2.1. Field Equations of Background Studies

Helmholtz free energy was given according to the free surface density of bone (Equation 1-3) \[4-7,10, 20, 21, 26\]. Related nomenclature was given in Table 1.

\[-\nabla \psi - \nabla \cdot \mathbf{J} - T_{ij} L_{ij} - \frac{1}{\beta} q_{i} \theta_{i} + h \geq 0 \quad (1)\]

\[\psi = \psi(\theta_{0}, \theta_{i}, S_{ij}, E_{ij}) = 0 \quad (2)\]

\[-\nabla \psi - \nabla \frac{\partial \psi}{\partial S_{ij}} S_{ij} - \frac{1}{\beta} q_{i} \theta_{i} + h \geq 0 \quad (3)\]

Rouhi et.al and others assumed that zero strain reference state at constant temperature situation \[4-7,10, 20, 21, 26\].

\[T_{ij}(\theta_{0}, 0, S_{ij}, \delta_{ij}) = 0 \quad (4)\]

In the reports it was assumed that strains were small and Equation 5-10 were reported \[3-7,10, 20, 21, 26, 27\].

\[e = \xi - \xi_{0} \quad (5)\]

\[E_{ij} = \frac{1}{2} (U_{ij} + U_{j,i}) \quad (6)\]

\[C = C(S_{ij}, E) \quad (7)\]

\[\psi = \phi(S_{ij}, E) \quad (8)\]

\[\frac{de}{dx} = \phi(S_{ij}, E) \quad (9)\]

\[\phi(S_{ij}, E) = \frac{C(S_{ij}, E) (\det(1+2E))^{1/2}}{\gamma} \quad (10)\]

In the investigations \(\phi(S_{ij}, E)\) and \(\psi(S_{ij}, E)\) were approximated by neglecting higher order terms in Taylor Series expansion and they were reported following equations (Equation 11-14) \[7\].

\[\phi(S_{ij}, E) \approx a(S_{ij}) + A_{ij}^{*}(S_{ij}) E_{ij} + \frac{1}{2} B_{ijkm}(S_{ij}) E_{ij} E_{km} \quad (11)\]

\[a(S_{ij}) = A_{ij}^{*}(S_{ij}, 0) \quad (12)\]

\[A_{ij}^{*}(S_{ij}) = \left[ \frac{\partial \phi(S_{ij}, E_{ij})}{\partial E_{ij}} \right]_{E_{ij}=0} \quad (13)\]

\[B_{ijkm}(S_{ij}) = \left[ \frac{\partial^{2} \phi(S_{ij}, E_{ij})}{\partial E_{ij} \partial E_{km}} \right]_{E_{ij}=0} \quad (14)\]
They developed the derivative form of the difference of unstrained volume fraction before remodelling (Equation 15-19) [7].

\[
\frac{de}{dt} = \{a(S_\lambda) + A_{ij}(S_\lambda)E_{ij}\}
\]

\[
\frac{de}{dt} = \{a_0 + a_1S_\lambda + a_2S_\lambda^2 + (A^0_{ij} + A_{ij}S_\lambda)E_{ij}\}
\]

\[A^0_{ij} = A^0_{ij}(0, E_{ij})\]

\[A_{ij} = \left[\frac{\partial A_{ij}(S_\lambda E_{ij})}{\partial S_\lambda}\right]_{S_\lambda = 0}
\]

\[A_{ij} = \left[\frac{\partial^2 \phi(S_\lambda E_{ij})}{\partial S_\lambda \partial E_{ij}}\right]_{E_{ij} = 0}
\]

Equation 20 referred to the bon remodeling process [4-7,10, 20, 21, 26, 27].

\[
\frac{de}{dt} = -\frac{dp}{dt} = A_{ij}S_\lambda(E_{ij} - E_{ij}^*)
\]

Active free surface density \((S_\lambda)\) of bone was reported in Equation 21 [7]. If the whole surface is effective for remodeling, thus \(\lambda\) equals to 1, and \(S_\lambda\) equals to \(S_B/V_t\) or \(S_v\) [4-7].

\[
S_\lambda = \lambda \frac{S_B}{V_t}
\]

Martin et al. reported that the specific surface increased with the rate of remodeling of bone. They gave Equation 22 and 23 to estimate the free surface density [4-7].

\[
\frac{de}{dt} = -\frac{dp}{dt} = A_{ij}(28.8P_v^5 - 101P_v^4 + 134P_v^3 - 93.9P_v^2 + 32.2P_v)(E_{ij} - E_{ij}^*)
\]

### Table 1. Nomenclature.

| Physical Properties            | Symbol |
|--------------------------------|--------|
| Helmholtz free energy          | \(\psi\) |
| Bulk density                   | \(\gamma\) |
| Volume fraction                | \(\nu\) |
| Specific entropy               | \(\eta\) |
| Absolute temperature, temperature | \(0, \theta_i\) |
| Stress tensor                  | \(T_{ij}\) |
| Kronoecker Delta               | \(\delta_{ij}\) |
| Velocity tensor (Gradient)     | \(L_{ij}\) |
| Strain Tensor, Strain (Equilibrium) | \(E_{ij}, E_{ij}^*\) |
| Displacement vector            | \(U\) |
| Displacement vector (Gradient) | \(U_{ij}\) |
| Surface Modeling Coefficient   | \(C\) |
| Function of active free surface density variation with strain | \(\phi\) |
| Heat flux vector               | \(q_i\) |
| Entropy                        | \(h\) |
| Active free surface density    | \(S_\lambda\) |
| Free surface density           | \(S_B\) |
| Difference between the initial and strained volume fractions | \(e\) |
| Initial volume fraction (Before the strain) | \(\xi\) |
| Material constants of bone     | \(a, a_0, a_1, a_2, A_{ij}^*, A_{ij}^0\) |
| Void Fraction (Porosity)       | \(P_v\) |
| Scattering Factor              | \(S_p\) |
2.2. Current Model and Results

In the literature, the importance of micro-strucural properties of bone was emphasized [2-32]. Some assumptions were made before the theoretical investigation. Wolff’s law was valid thus the bone matrix’s condition was depend on strain tensor history [9]. There was not any bone disease so blood plasma supplied the materials for the synthesis of bone matrix. Bone matrix established a suitable environment for the required mass transfer to the osteoblasts and osteoclasts. Proposal of Beaupre et al. was valid in the equilibrium condition, if \( E_{ij} = E_{ij}^* \) bone remodeling was interrupted [21]. Also we assumed that bone remodeling could only occur in the presence of an active surface area [4-7]. Morphological and functional characteristics of the bone surface allow us to evaluate its free energy. Five different Archimedean lattice models (\( 3^6, 4^4, 6^3, 4,8^2, 3,12^2 \)) which bond and site percolation thresholds were known from the literature were used [33, 38]. Because the bond percolation threshold allowed us to determine the potential lattice which might be promising for bone remodeling. Circumferential lengths were adjusted to the same size, thus all polygons had 404 \( \mu \text{m} \) equal perimeter. (Figure 2) Distances of the channels were fixed to 10 \( \mu \text{m} \) for whole polygons. To derive our novel equation for different surface patterns (on 1x1 mm\(^2\) total planar area), it was assumed that polygons had been filled with bone, blood plasma was supposed to flow through micro-channels and they formed a porosity.

![Figure 2. Schematical representation of perimeters for Archimedean lattice models.](image)

AFSD ratios were estimated in the range of 0.71- 0.8498 for different Archimedean lattice models (Figure 3). The minimum void fraction was calculated about 0.18. Our AFSD results were found consistent with Lerebourgs et al.’s investigation [39], also our theory explained their scattered results. 3\(^6\) lattice has a greater potential because of its high specific surface and minimum bond percolation threshold. Different AFSD ratios can be obtained with lattices which have the same void fraction such as 3\(^6\) and 4\(^4\) (Figure 3 right). AFDS ratio of 4\(^4\) was calculated lower than 3\(^6\). This situation reduces its potential for bone remodeling. This result can be attributed to the reduced micro-flow or signal transmission due to vertices of the porosity. A scattering (dispersion error) factor (S\(_F\)) should be added to calculate more accurate values according to the coordination number of the lattices (Figure 3 left). If coordination number equals to 6, Equation 24 should be used. If it is below from 6, Equation 25 should be used.

\[
\frac{dE}{dt} = \frac{dP_v}{dt} = A_{ij}(18.355P_v^5 - 46.79P_v^4 + 33.85P_v^3 - 8.816P_v^2 - 1.5P_v)(1/S_F)(E_{ij} - E_{ij}^*) \quad (24)
\]

\[
\frac{dE}{dr} = \frac{dP_v}{dr} = A_{ij}((18.355P_v^5 - 46.79P_v^4 + 33.85P_v^3 - 8.816P_v^2 - 1.5P_v)(S_F))(E_{ij} - E_{ij}^*) \quad (25)
\]
3. Conclusions

In the scope of this paper, AFSD Maps were presented and a novel equation was proposed. $3^6$ and $4^4$ lattices were suitable for bone remodeling. Scattering factor will be beneficial for precise computation of AFSD values which have irregular dispersion. This study is a preliminary investigation and further studies are necessary to evaluate the maximum AFSD ratio of other three dimensional lattices.

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