Alignment of Rods and Flakes using Electric Field

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Abstract

Electrically neutral anisotropic objects can be aligned by the applied electric field. The required processing conditions include to submerge the objects in a matrix with higher electrical conductivity than that of the objects and to apply electric field to the suspension. The objects may be in rod, disk, flakes or other anisotropic shapes. Carbon nanotubes, silicon nanowires, micro coils, DNA and many bacteria can be approximated as rod-like shape, and graphene can be considered as a shape of flake. A fundamental investigation to this phenomenon has been carried out in the present work. Numerical calculation based on thermodynamics shows a confirmative trend to use electric field to align those materials. The driving force in the alignment processing is an equivalent configuration force dependent on the discrepancy between the electrical properties of the anisotropic particles and matrix. Copyright © VBRI Press.

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Introduction

The fabrication of many functional devises requests to align the anisotropic shaped materials. This is because the materials with anisotropic shape often possess anisotropic mechanical, electrical, magnetic and optical properties but a randomly oriented configuration will cancel the desirable anisotropic properties in overall scale. The applications can be seen in censors, switches [**1**], memory electronics [**2**], display devices [**3**] and many other cases. The aligned carbon nanotubes are desirable in the replacement of the damaged nerves in biological experiments [**4**]. The aligned graphene is desirable in surface coating [**5**]. Carbon nanotube is a rod-like geometry. Graphene is thin flake-like geometry. The aligned nanocones has high magnitudes of conductivity [**6**] for the fabrication of thermal rectifier [**7**]. The aligned silicon nanowires have advanced optical properties [**8**]. The aligned micro-coils help to generate remarkable conductivity [**9**]. Alignment of micro-scale and nanoscale rods and flakes has potential applications and, therefore, has attracted significant research interests [**10**].

The fundaments in using of electric field to align the rods and flakes are explored in the present work. The materials to be aligned are electrically neutral objects with negligible polarization. This means that the mechanism of using electric field to align the rods and flakes is different from that in conventional electrophoresis or dielectrophoresis [**11-12**]. The force to align the rods and flakes is a configuration force derived from the thermodynamics [**13**]. The initial notification of the alignment effect of the passing electric current in a matrix with submerged objects can be traced back to 30 years ago where an experiment shows that the growing of crystals in liquid metal has been elongated along the direction of electric field by the passing electric field [**14**]. This is again noticed in our own experiments that the shape of inclusions has been changed toward the electric field direction during the solidification of liquid steel [**15**]. Further experiments confirm the alignment effect of the electric current on the crystals at ambient environments, where the crystallographic texture in steels can been altered by the electric field [**16**]. The orientation of cementite phase (Fe_3C) in low-carbon steel has been observed to be changed and aligned along the electric field direction, and the alignment can be re-organized if the external electric field changes its direction [**17**]. More recently, the alignment effects of electric field have been implemented to the fabrication of purposely aligned structural materials [**18**].

In our previous study, a torque has been discovered in the calculation of the effect of electric field on the disc-like particles [**19**]. The magnitude of the torque is significant even when the electric field gradient is in a scale of 1 v/cm. It provides a strong indication that the electric field can be used to align the disc-like particles. The aim of the present work is to investigate the effect of electric field on the alignment of rods and flakes. Abundant materials are in these shapes.

Experimental

The experimental setting up includes to put the rods or flakes into a fluid matrix to form suspension. The matrix should have higher electrical conductivity than that of the objects to be aligned and the two phases should be immiscible to prevent the particles to be dissolved during the alignment treatment. Ideally the container for the fluid should have a length which is much larger than that of in cross section in order to minimize the surface effect near to the ends of electrodes. The direction of electric field should be along the longest dimension. The matrix can be in liquid or conductive gas. The magnetic permeability of the liquid can be the same or different from that of the anisotropic particles. In the present study, one uses the conductivity of 1.22×10^6 S·m^{-1} and magnetic permeability of $30\mu_0$ for the anisotropic material, where μ_0 is the vacuum permeability. These values are taken from that of the cementite where some experiments have been done in our laboratory for this phase [**17, 20-21**]. The electrical conductivity for the matrix is assumed to be 9.17×10^6 S·m^{-1} and its magnetic permeability is assigned to 300 μ_0. These values are taken from the ferrite phase in steel at ambient temperature [**22, 23**]. The dimension ratio of liquid matrix is defined as 20:9:8 in three Cartesian coordinates. Electric field is applied along the longest dimension of the system. The applied electric potential is 20 volts. 100 anisotropic particles are injected into the liquid matrix for the alignment. The volume fraction of all the anisotropic particles in the system is 10.42%.

The experimental results on the using of an electric field to align the anisotropic microstructure are demonstrated in **Fig. 1**. The system contains two phases with the volume fraction of the submerged phase as well as the electrical and magnetic properties are in the values of earlier described. The only difference is that the matrix is not a fluid but a solid. The alignment is not via a mechanical rotation of the anisotropic phase but a chemical reorganization of the microstructure. The microstructure of the materials has no detectable orientation before the electrical treatment, as can be seen in **Fig. 1(a)**. When 20 volts electrical potential has been applied to the materials for 1000 times in a frequency of 1 Hz and loading duration of each time at 20 μs the aligned microstructure has formed. This can be seen clearly in **Fig. 1(b)**. The detailed sample preparation methods are presented in our earlier publications [**17, 21**].

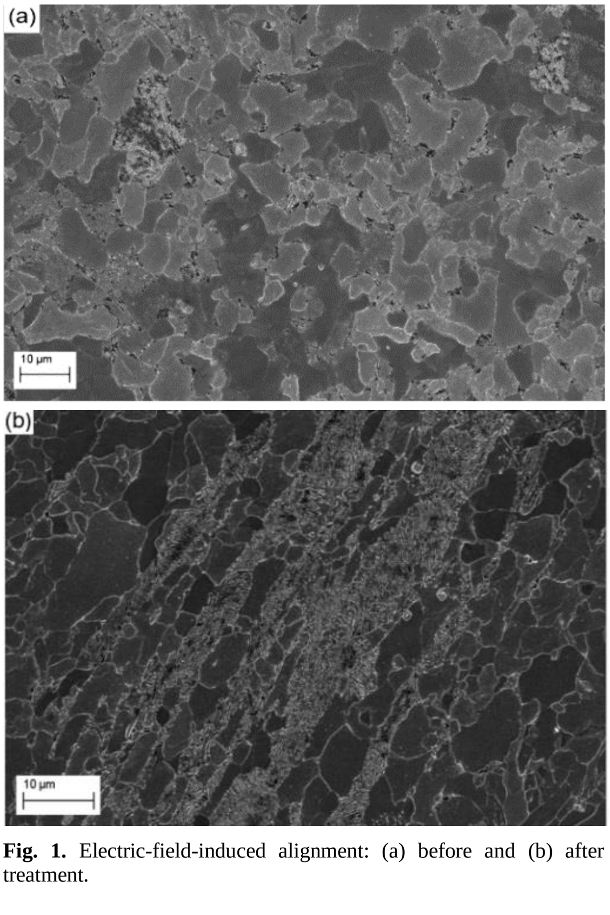

Fig. 1. Electric-field-induced alignment: (a) before and (b) after treatment.

Results and discussion

Putting 100 anisotropic rods in to the conductive matrix randomly, the configuration of system is demonstrated in **Fig. 2(a)**. The colors represent the geometric orientations. The configuration is obtained by numerical calculation using a mechanism like phase-field model [**24**]. The system initially contains 100 randomly distributed nucleation sites and then the particles to grow in a speed ratio of 10:1:1 along three principle axes along individual particle's coordinates [**25**]. The growth is suspended when the total volume of all particles reaching to the defined fraction. After the alignment processing, it is desirable that all the rods are oriented along the direction of electric field, as presented in **Fig. 2(b)**. The color of the rods are almost the same but with some slightly fluctuations. The criteria to judge whether the configuration in **Fig. 2(b)** can be achieved by applied electric field from that of **Fig. 2(a)** is the thermodynamics. There is no obvious force presented because the particles are in electrically neutral and assumed to be not polarized. From the thermodynamic point of view, the alignment processing does not include any phase transition and hence the system chemical free energies in **Fig. 2(a)** and **(b)** are identical. There is no agglomeration and break down of rods included and hence the total interface energy in both cases are identical. The stress-strain energy can be quickly released due to the fluidity of the matrix. The only difference that contributes to the alignment is the electric current free energy. According to the theory, the electric current free energy G_e is defined as [**13**]

$$G_e = -\frac{1}{8\pi}\iint \frac{\mu(r)\vec{j}(r)\cdot\vec{j}(r')}{|r-r'|}drdr' \tag{1}$$

where μ(r) is the magnetic permeability of materials at space position *r*. $\vec{j}(r)$ is the electric current density at position *r*. The integration goes throughout the volume of the system. The judgment for whether electric potential could align the randomly oriented rods is to find out whether the electric current free energy in **Fig. 2(b)** is less than that of **Fig. 2(a)**.

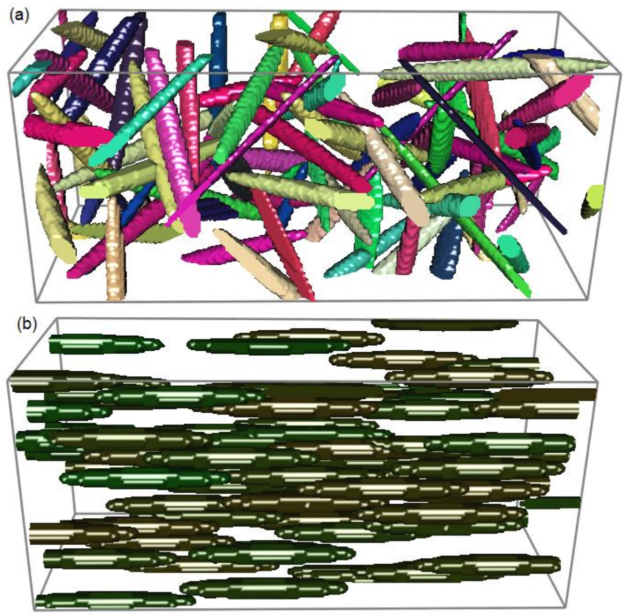

Fig. 2. 100 rods with a total volume fraction 10.42% in a matrix: (a) in random distribution; (b) aligned along the direction of electric field.

In order to calculate the electric current free energy according to Eq. (1), one needs to get the electric current distribution in the system when the rods are distributed in various ways. This can be done by the relaxation method using the provided electrical conductivity of anisotropic particles and the liquid matrix. The detailed derivation of using relaxation method in calculation of the electric current distribution at steady state has reported before [**13**]. In the present case, the system is represented by 200 × 90 × 80 lattice. For a lattice distance of 10 nm, the obtained magnitude of electric current density distribution for the configuration in **Fig. 2(a)** is presented in **Fig. 3(a)** and that for the configuration demonstrated in **Fig. 2(b)** is demonstrated in **Fig. 3(b)**. The unit for the electric current density is 10^{-3} A/nm^2. The data was plotted using an in-house software MatVisual. The color spectrum represents the magnitude of the current density. It can be seen that the electric current density distribution is very different when the configuration of the rods are different. The orientations of the rods affect the electric current distributions and hence the electric current free energy. According to the calculation, the electric current free energy for the random orientation of the rods demonstrated in **Fig. 2(a)** is -2.3653×10^{-07} J while that for the aligned configuration illustrated in **Fig. 2(b)** is -2.75942×10^{-07} J. Clearly, the alignment of the rods from the initial randomly orientation reduces the electric current free energy. The system free energy reduces along with the electric current free energy while the chemical free energy, interface energy and strain-stress energy are not changed in the processing. According to the second law of thermodynamics, the configuration in low system free energy state is preferred. Therefore, the electric field induces the rods to align along the electric field direction.

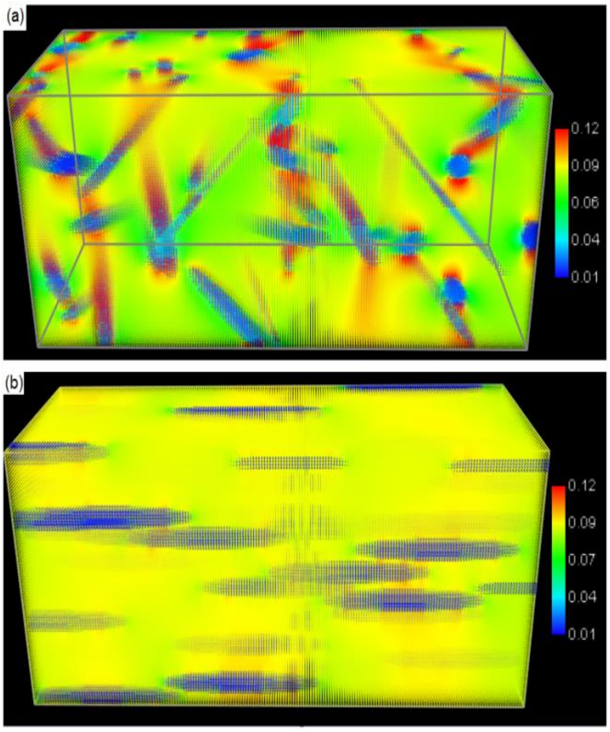

Fig. 3. The electric current density in a matrix containing 100 rods at (a) randomly distribution and (b) aligned along the direction of electric field.

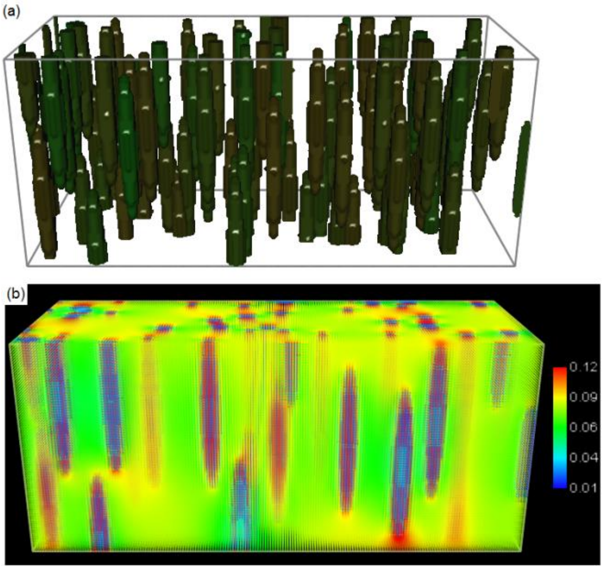

Fig. 4. (a) 100 rods are aligned to a direction in perpendicular to that of the electrical field and (b) the correspondence electric current density distribution.

Is it possible to align the rods into other direction rather than along the direction of electric field? To answer this question, another aligned configuration is calculated. The configuration and the electric current density distribution are presented in **Fig. 4(a)** and **4(b)** respectively. According to the calculation, the electric current free energy for the configuration in **Fig. 4(a)** is -2.31738×10^{-07} J, which is even higher than the random configurations in Figure 2(a). Therefore, it is not possible to align the rods in other directions than that of the electric field.

It can be seen clearly from **Fig. 3** that when the rods are parallel to the direction of electric field the current density inside the high electrical resistivity rods is low (blue). However, when the rods are perpendicular to the electric field a lot of high current density areas both inside the rods and between rods are observed, as can be seen from **Fig. 4(b)**. The high heterogeneous current distribution corresponds to the high electric current free energy according the calculations in the present work. The eddy current intends to drive the rods to rotate to parallel to the electric field. It is also know that the high local current density will produces high Ohm heat. The rods at different orientations will cause different temperature rising when the electric current is passing by. This agrees with our other published calculations [**19**].

The similar calculations have been performed to the configurations of flakes that are demonstrated in **Fig. 5**. The electric current free energy in the aligned structure shown in **Fig. 5(b)** is lower than that of **Fig. 5(a)** and hence is preferred. Electric current induces the flakes to align along the direction of electric field.

In the electric field induced alignment processing, the differences of electrical properties between the matrix and anisotropic objects play the most important role. Larger difference produces higher efficiency. In the current calculation, only the case when the electric conductivity of anisotropic objects is higher than that of the matrix has been considered. Other cases will be considered in the future. The method is more effective when the magnetic permeability of the system is larger. The electric current free energy is proportional to the square of the magnitude of electric field.

Fig. 5. 173 flakes in (a) random distribution and (b) aligned along the direction of electric field.

Conclusion

A method to align rods and flakes has been investigated and developed. It is suggested to put the anisotropic shaped objects to a fluid matrix to form suspension. The matrix should have higher electrical conductivity than that of the anisotropic inclusions. An electric field is applied to the system by putting two electrodes to the matrix and allow the electric field along the longest dimension of the system. The aligned system has lower electric current free energy and hence the lower system free energy. The processing is examined from the thermodynamic point of view.

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Author's contributions

Authors have no competing financial interests.

Supporting information

The figures are generated by plotting the numerical calculations using MatVisual software.

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