

Towards minimal negative static electric susceptibility: crystal engineering in active metamaterials

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Abstract—This study examines materials with negative static electric susceptibility, emphasizing their structural dependencies and critical bounds. Using simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc) lattices, the static electric susceptibility is calculated via the Clausius-Mossotti equation. The results reveal that bcc and fcc lattices achieve more favorable bounds than sc lattices, making them suitable for isotropic active metamaterials. These findings provide insights into optimizing material properties for applications like electrostatic levitation.

I. INTRODUCTION

The exploration of materials exhibiting negative static electric susceptibility $\chi^{(0)} < 0$ presents a transformative opportunity in the field of active metamaterials [1]. Negative static electric susceptibility, a property associated with systems not in thermodynamic equilibrium [2]–[5], has been identified as a critical enabler for phenomena such as electrostatic levitation [6], [7]. In a previous study, a theoretical basis has been provided which establishes the possibility of $\chi^{(0)} < 0$ in non-equilibrium material [6]. Here, the study investigates the structural dependencies and critical bounds of $\chi^{(0)}$ to establish the most suitable configurations for achieving minimal $\chi^{(0)}$ in isotropic active metamaterials.

II. MODEL AND METHODOLOGY

The study models materials composed of identical, point-like, dipolarizable entities arranged in periodic structures. These entities are characterized by linear, isotropic responses to local electric fields. The static electric susceptibility $\chi^{(0)}$

TABLE I
NORMALIZED PRIMITIVE LATTICE VECTORS

	sc	bcc	fcc
$\tilde{\mathbf{a}}_1$	$\hat{\mathbf{x}}_1$	$(1/2^{2/3})(-\hat{\mathbf{x}}_1 + \hat{\mathbf{x}}_2 + \hat{\mathbf{x}}_3)$	$(1/2^{1/3})(\hat{\mathbf{x}}_2 + \hat{\mathbf{x}}_3)$
$\tilde{\mathbf{a}}_2$	$\hat{\mathbf{x}}_2$	$(1/2^{2/3})(\hat{\mathbf{x}}_1 - \hat{\mathbf{x}}_2 + \hat{\mathbf{x}}_3)$	$(1/2^{1/3})(\hat{\mathbf{x}}_1 + \hat{\mathbf{x}}_3)$
$\tilde{\mathbf{a}}_3$	$\hat{\mathbf{x}}_3$	$(1/2^{2/3})(\hat{\mathbf{x}}_1 + \hat{\mathbf{x}}_2 - \hat{\mathbf{x}}_3)$	$(1/2^{1/3})(\hat{\mathbf{x}}_1 + \hat{\mathbf{x}}_2)$

relates to the static polarizability α through the Clausius-Mossotti equation [6]:

$$\chi^{(0)} = \frac{4\pi\tilde{\alpha}}{1 - \frac{4\pi}{3}\tilde{\alpha}}, \quad (1)$$

where $\tilde{\alpha} = N\alpha/(4\pi\epsilon_0)$ is the dimensionless reduced static polarizability, N is the number of entities per unit volume, and ϵ_0 is the permittivity of free space. It is found that any set of two or more entities (assuming the entities are located at distinct positions) has an upper critical value of $\tilde{\alpha}$, which we denote $\tilde{\alpha}_{c+}$, and a lower critical value of $\tilde{\alpha}$, which we denote $\tilde{\alpha}_{c-}$, such that: if $\tilde{\alpha}_{c-} < \tilde{\alpha} < \tilde{\alpha}_{c+}$ then the system is stable, and if $\tilde{\alpha} < \tilde{\alpha}_{c-}$ or $\tilde{\alpha} > \tilde{\alpha}_{c+}$ then the system is unstable [6]. The method first involves determining $\tilde{\alpha}_{c+}$ and $\tilde{\alpha}_{c-}$ for finite numbers of entities in arbitrary positions, later extending to infinite sc, bcc, and fcc crystal lattices. Fig. 1 illustrates the finite cubic crystals defined by the reduced primitive lattice vectors. The normalization factors, $1/2^{2/3}$ and $1/2^{1/3}$, for the bcc and fcc cases are chosen respectively such that the primitive cells are of unit volume. This means that the number density is the same in each of the sc, bcc, and fcc cases and given by $N = 1/a^3$ (a is the length of the sc cell edge), which is convenient for our purposes to compare the resulting critical values of $\tilde{\alpha}$ in a like-for-like fashion.

III. RESULT AND DISCUSSION

Plots of the points $(1/n^2, \tilde{\alpha}_{c\pm, n})$ are shown in Fig. 2 which not only indicates the trend of the reduced critical values of polarizability against increasing crystal size n but also indicate how the limiting values $\tilde{\alpha}_{c\pm, \infty}$ may be determined by extrapolation. It can be seen that the values of $\tilde{\alpha}_{c+, n}$ decrease with increasing n in each of the sc, bcc, and fcc cases, whereas the values of $\tilde{\alpha}_{c-, n}$ increase with increasing n . Again, in both the positive and negative cases, the values of $\tilde{\alpha}_{c-, n}^{\text{bcc}}$ and $\tilde{\alpha}_{c-, n}^{\text{fcc}}$ become increasingly coincident with each other as n increases, whereas the values of $\tilde{\alpha}_{c-, n}^{\text{sc}}$ remain significantly

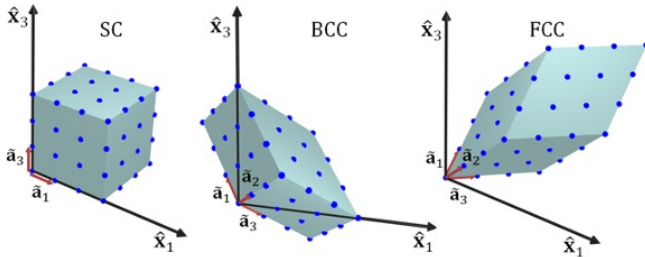


Fig. 1. Finite cubic crystals defined by the respective (reduced) primitive lattice vectors $\tilde{\mathbf{a}}_1$, $\tilde{\mathbf{a}}_2$, and $\tilde{\mathbf{a}}_3$ tabulated in Table I. Here, $\hat{\mathbf{x}}_1$, $\hat{\mathbf{x}}_2$, and $\hat{\mathbf{x}}_3$ are the (dimensionless) unit vectors of a conventional Cartesian system.

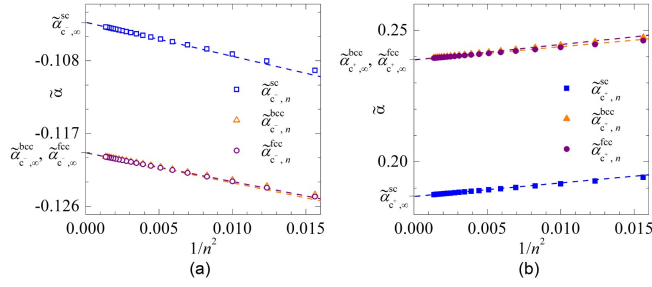


Fig. 2. Plots of the points $(1/n^2, \tilde{\alpha}_{c\pm, n})$ are seen to be approximately linear. (a) Negative critical values and (b) positive critical values of reduced static polarizability $\tilde{\alpha}$.

different. We also see that the plots are approximately linear in each case; this enables the best estimates for the values of $\tilde{\alpha}_{c\pm, \infty} = \lim_{n \rightarrow \infty} \tilde{\alpha}_{c\pm, n}$ to be determined as the vertical intercepts of linear fit lines. The values obtained by this method are listed in Table II. The critical values of the static electric susceptibility $\chi_{c\pm}^{(0)}$ are determined by inserting the values of $\tilde{\alpha}_{c\pm, \infty}$ into Eq. (1). The values of $\chi_{c\pm}^{(0)}$ thus obtained are also listed in Table II to three significant figures. The results of the study are summarized in Fig. 3.

TABLE II
EXTRAPOLATED CRITICAL VALUES OF THE REDUCED STATIC POLARIZABILITY $\tilde{\alpha}_{c\pm, \infty}$, AND THE ASSOCIATED CRITICAL VALUES OF THE STATIC ELECTRIC SUSCEPTIBILITY $\chi_{c\pm}^{(0)}$, FOR SC, BCC, AND FCC INFINITE CRYSTALS, STATED TO THREE SIGNIFICANT FIGURES.

	sc	bcc	fcc
$\tilde{\alpha}_{c+, \infty}$	0.187	0.239 $\left[\frac{3}{4\pi}\right]$	0.239 $\left[\frac{3}{4\pi}\right]$
$\tilde{\alpha}_{c-, \infty}$	-0.103	-0.119 $\left[-\frac{3}{8\pi}\right]$	-0.119 $\left[-\frac{3}{8\pi}\right]$
$\chi_{c+}^{(0)}$	10.8	$[\infty]$	$[\infty]$
$\chi_{c-}^{(0)}$	-0.906	-1.00 $[-1]$	-1.00 $[-1]$

IV. CONCLUSION

The lower bound of $\chi^{(0)}$ is inherently dependent on the crystal structure, exhibiting distinct values for sc lattices compared to bcc and fcc arrangements. Consequently, determining the lower bound for a given crystal structure is a complex problem that, in general, can only be rigorously addressed through the analytical approach employed in this study [6]. Notably, this indicates the absence of a universal, structure-independent derivation for the lower bound.

While our assumption of point-like dipolarizable entities may introduce certain limitations when applied to real-world systems, the results affirm the structural dependence of $\chi^{(0)}$. Specifically, they demonstrate that bcc and fcc lattices are more favorable for designing isotropic active metamaterials with minimal $\chi^{(0)}$. The exact lower bounds for sc differ from those for bcc and fcc structures, providing a pathway for optimizing material properties. These findings hold promise

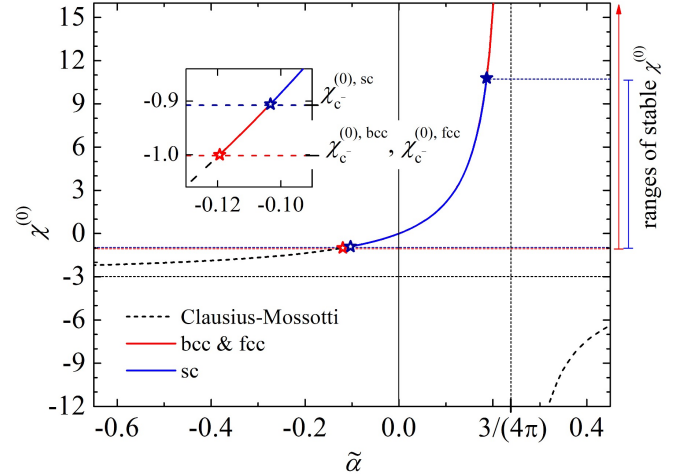


Fig. 3. Plot of the static electric susceptibility $\chi^{(0)}$ of the material as a function of the reduced static polarizability $\tilde{\alpha}$ of the dipolarizable entities from which the material is composed, according to the model.

for advancements in electrostatic levitation and other novel applications. Theoretical studies on electrostatic levitation over a bowl-shaped medium [4] provide a foundation for organizing active meta-atoms to achieve this yet-to-be-realized phenomenon.

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