Effective medium theory with hybrid impacts of phase symmetry and asymmetry

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I. Introduction

Phase transitions are common in nature, during which the macroscopic physical properties of the system might change significantly. People have used this phenomenon to achieve various applications, such as smart windows [1], energy storage [2], and thermal diodes [3]. Recent research found a hysteresis phenomenon of electric conductance against metallic phase ratio during the thermally driven metal-insulator transition in the vanadium trioxide (V_2O_3) system [4]. Profoundly exploring the hysteresis mechanism might help analyze the phase transition behavior, which guides controlling thermal hysteresis magnitude for practical applications. Due to successful applications of the effective medium theory (EMT) in predicting the macroscopic physical quantities of composites [5,6], we develop an EMT theory to study the hysteresis mechanism in this work.

II. Theoretical analysis

Maxwell-Garnett (M-G) formula and Bruggeman formula are fundamental in EMT, with symmetrical and asymmetrical characteristics, respectively [6]. We apply them to calculate the effective electric conductance G_e of the sample in this study.

The M-G formula is suitable for solving the situation where inclusions are embedded in a host [6], as shown in fig. 1(a). For a two-dimensional isotropic binary composite, the M-G formula is

$$\frac{G_{\mathrm{e,M-G}}-G_{\mathrm{h}}}{G_{\mathrm{e,M-G}}+G_{\mathrm{h}}}=f_{\mathrm{i}}\frac{G_{\mathrm{i}}-G_{\mathrm{h}}}{G_{\mathrm{i}}+G_{\mathrm{h}}},$$

where $G_{\mathrm{e,M-G}}$ is the effective electric conductance calculated by the M-G formula; G_{i} is the electric conductance of the inclusions; G_{h} is the electric conductance of the host; f_{i} is the area ratio of the inclusions [6]. It is asymmetrical during the warming and cooling processes.

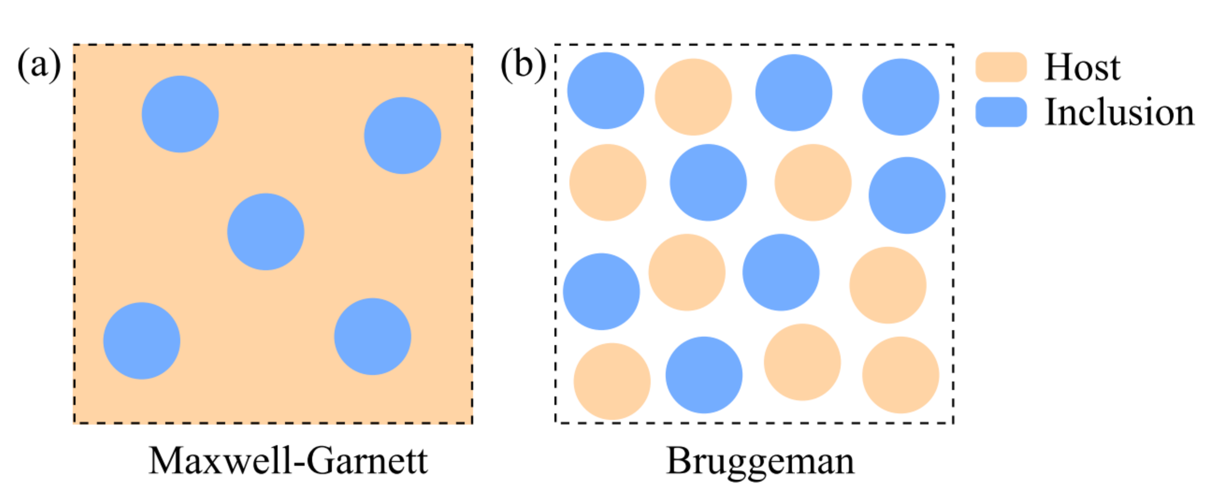

Fig. 1: Schematic diagram of (a) Maxwell-Garnett (M-G) formula for phase asymmetry and (b) Bruggeman formula for phase symmetry [6].

The Bruggeman formula is suitable for solving the situation where the inclusions and host are exchangeable [6], as shown in fig. 1(b). For a two-dimensional isotropic binary composite, the Bruggeman formula is

$$f_{\mathrm{i}}\frac{G_{\mathrm{i}}-G_{\mathrm{e,B}}}{G_{\mathrm{i}}+G_{\mathrm{e,B}}}+f_{\mathrm{h}}\frac{G_{\mathrm{h}}-G_{\mathrm{e,B}}}{G_{\mathrm{h}}+G_{\mathrm{e,B}}}=0,$$

where $G_{\mathrm{e,B}}$ is the effective electric conductance calculated by the Bruggeman formula; f_{h} is the area ratio of the host; $f_{\mathrm{i}} + f_{\mathrm{h}}$ = 100% [6]. It is symmetrical during the warming and cooling processes.

Capturing the characteristics of the nucleation and growth behavior of the minority phase in the majority phase during the warming (cooling) process, we treat the inclusion and host in the above two formulas as metallic (insulating) and insulating (metallic) phases, respectively. By combining the M-G and Bruggeman formulas, we finally obtain G_e.

III. Experimental fitting

We now verify the above theory. We plot the relationship between G_e and metallic phase ratio f_{met}. When f_{met} rises from 0% to 50%, the electric conductance difference $\Delta G_e(f_{\mathrm{met}})$ in the warming and cooling processes increases and then decreases. A similar and more significant phenomenon occurs when f_{met} rises from 50% to 100%. It reproduces the hysteresis of G_e against f_{met} in ref. [4].

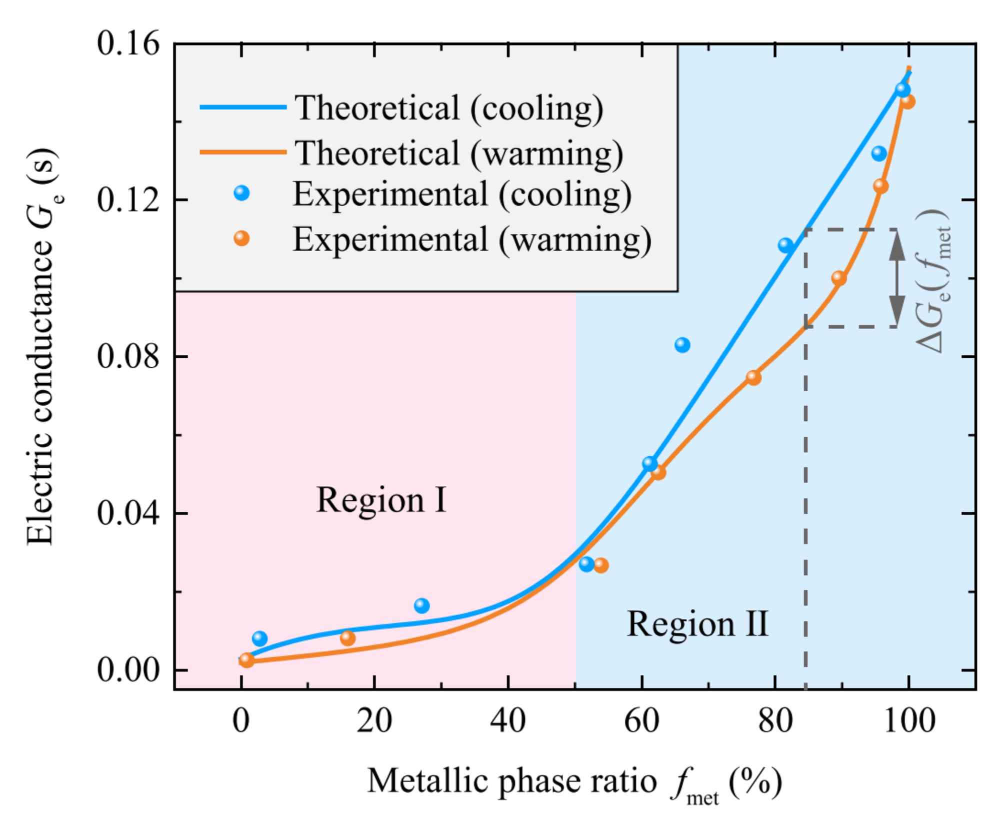

Fig. 2: Relationships between G_e and f_{met} in the warming and cooling processes. The experimental data is extracted from ref. [4].

IV. Summary

In summary, we established an effective medium theory to predict the relationship between the effective electric conductance G_e and metallic phase ratio f_{met} during phase transition in the V_2O_3 system. It reveals that the hysteresis of $G_e(f_{\mathrm{met}})$ is due to the hybrid impacts of phase symmetry and asymmetry in spatial distribution. This theory can be applied to study the dynamic behavior of the nucleation and growth process during phase transition for further study.

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