

## **Phase Transformation Behavior of C60 Fullerene under Atmospheric Pressure**

**Wen-Hwa Chen, Chun-Hung Wu and Hsien-Chie Cheng**

### **Summary**

The phase transformation behaviors of C60 fullerene under atmospheric pressure are reported using a proposed thermostat molecular dynamics method designed for a solid system. We find that C60 fullerene directly undergoes a solid-vapor phase transformation, instead of a solid-liquid phase transition, at a specific threshold temperature. It reveals that C60 fullerene will sublime when heated rather than melt under atmospheric pressure. This phenomenon is coincident with that of graphite at pressures below 10MPa. The sublimation point of C60 fullerene, rather than the melting, is about 4350o20K, locating in the published range of about 4000-4500K for graphite at pressures below 10 MPa.

