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Citation: Chin. Phys. B, 2026, 35 (**6**): 068101. DOI: 10.1088/1674-1056/ae5172
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RAPID COMMUNICATION

Influence mechanism of temperature fluctuation on the growth of adjunct diamond under HPHT conditions

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(Received 26 January 2026; revised manuscript received 10 March 2026; accepted manuscript online 13 March 2026)

The growth of adjunct crystals significantly impacts the quality of synthetic diamonds, with temperature fluctuations being the primary cause. This study investigates the influence mechanism of temperature fluctuations on the growth of synthetic diamond crystals under high temperature and high pressure (HPHT) conditions through a combination of experimental and numerical simulation approaches. Numerical simulations reveal that ambient temperature variations directly affect the temperature field within the cavity, subsequently altering the carbon solubility in the metal catalyst. Over time, the synthesis process, influenced by varying solubility due to temperature changes, leads to secondary diamond growth, resulting in the formation of adjunct diamonds. This study offers a theoretical explanation of how temperature fluctuations affect the growth of these crystals, providing valuable theoretical guidance for the experimental synthesis of high-quality diamonds in industrial settings.

Keywords: high temperature and high pressure (HPHT) method, adjunct diamond, temperature fluctuation

PACS: 81.05.ug, 07.35.+k

DOI: 10.1088/1674-1056/ae5172 **CSTR:** 32038.14.CPB.ae5172

1. Introduction

High-quality synthetic diamonds, due to their outstanding physical and chemical properties such as excellent chemical inertness,[1] high thermal conductivity,[2] high carrier mobility,[3] ultra-wide band gap,[4] and wide spectral transmittance,[5] are widely used and highly regarded in numerous fields, including precision processing,[6–8] electronics,[9,10] optics,[11,12] quantum communication[13,14] and semiconductors.[15–17] The high temperature and high pressure (HPHT) method stands as one of the predominant techniques for synthetic diamond production. The core principle involves utilizing high-pressure equipment to generate ultra-high pressure and temperature, which catalyze the transformation of graphite into a diamond structure through metallic catalysts.[18–20] The HPHT method offers advantages such as high production efficiency and relatively controllable costs, enabling the fabrication of synthetic diamonds in various sizes and qualities to meet diverse demands in industrial production and scientific research.[21,22]

The temperature field uniformity within the HPHT diamond synthesis cavity plays a critical role in diamond crystal growth.[23,24] In practical synthesis environments, temperature fluctuations caused by day-night cycles and weather changes significantly disrupt the cavity's temperature distribution, ultimately affecting diamond nucleation and growth kinetics. During synthesis, unexpected secondary crystallization often occurs on crystal surfaces, forming adjunct crystal structures. This phenomenon severely impacts the mechanical, optical, and electrical properties of diamonds. Therefore, controlling the growth of adjunct crystal structures has become a key challenge in improving the quality and purity of synthetic diamonds. Although the effects of pressure,[25,26] temperature[27,28] and catalyst composition[29,30] on the growth of diamond have been studied, the mechanism of how the fluctuation of ambient temperature affects the formation of adjunct diamond crystals is still unclear.

This study investigates the influence mechanism of temperature fluctuations on the growth of adjunct diamond crystals under HPHT conditions through a combination of experimental and numerical simulation approaches. By conducting diamond synthesis experiments under different ambient temperature conditions and simulating the temperature field

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within the catalyst using finite element analysis, this study aims to provide a theoretical explanation for the observed phenomena. The results are expected to offer valuable insights into the role of temperature fluctuations in the formation of synthetic crystals and to provide guidance for optimizing the HPHT synthesis process to produce high-quality synthetic diamonds.

2. Experimental and simulation details

The diamond synthesis experiment was conducted in a Chinese-type cubic high-pressure apparatus (CHPA) with a sample assembly size of 42 mm×42 mm×42 mm, using an alloy catalyst under 5.7 GPa and 1260 °C. The structure of the high-pressure apparatus and the assembly of the synthetic sample cavity are shown in Fig. 1. High-purity graphite powder and Ni–Mn–Co alloy were used as the carbon source and catalyst, respectively. A diamond with a well-formed {100} crystal face of 0.5 mm×0.5 mm was used as the seed crystal. After the HPHT experiment, the synthesized diamond was dissolved in a thermal mixture of nitric acid and sulfuric acid to remove residual impurities on the crystal surface. The morphology of diamond crystals synthesized under the condition of temperature difference was observed by optical microscopy.

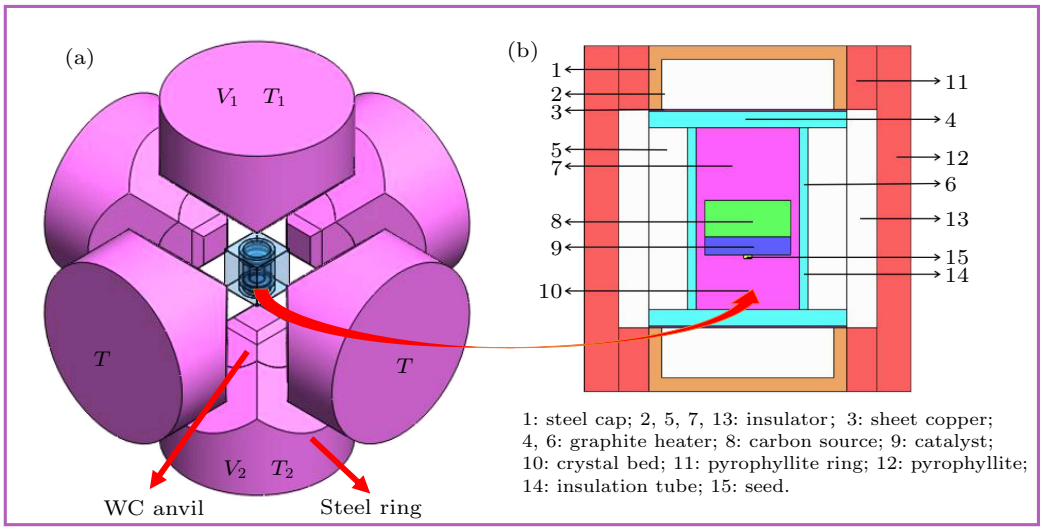


Fig. 1. (a) High-pressure apparatus structure. (b) Assembly of the synthetic sample cavity.

The thermal coupling module of ANSYS multi-field coupling analysis software was used to simulate the temperature field of the catalyst. The bottom cylinder block of the CHPA is in contact with the ground and is most affected by the external ambient temperature, especially in rain and snow weather with a large temperature difference between day and night. Therefore, according to the measured results of the temperature of the underside of the steel rings, we set the thermal analysis boundary conditions of the nodes at different times (corresponding to different time steps) when the external ambient temperature changes, as shown in Table 1. The voltage V_1 was set to 2.58 V and voltage V_2 was set to 0 for all experiments. The material parameters used in the simulation can be found in the relevant literature.[31,32]

Table 1. Thermal analysis boundary conditions.

Time steps	Underside temperature of six steel rings (°C)					
	Top (T_1)	Bottom (T_2)	Left	Right	Front	Back
0 s–400 s	50	50	50	50	50	50
400 s–800 s	50	10	50	50	50	50
800 s–1000 s	50	50	50	50	50	50
1000 s–1200 s	50	20	50	50	50	50
1200 s–1600 s	50	50	50	50	50	50

3. Results and discussions

3.1. Experimental results of diamond synthesis

Figure 2 shows the experimental results of large diamond single crystals synthesized under different ambient temperature fluctuations. The position marked by the red curve is the adjunct crystal formed by secondary growth. It can be observed from the figure that the diamond crystal shape is not complete, and secondary growth occurs in the local area of the crystal, leading to the formation of an adjunct diamond crystal. The degree of crystallization of synthetic crystals is affected by the temperature difference of the environment. As can be seen from the figure, the crystals in Figs. 2(a)–2(c) are secondary crystalline crystals produced when the ambient temperature fluctuation is not large, and secondary crystalline crystals can maintain a certain crystal type. The crystals in Figs. 2(d)–2(f) are secondary or multiple crystalline crystals produced when the ambient temperature fluctuates greatly. The secondary or multiple crystalline crystals formed are relatively dense and the crystal form is incomplete. The experimental results show that the greater the temperature fluctuation, the more secondary crystals grow, and the poorer the quality of

the crystals. The growth of secondary crystals is significantly influenced by temperature fluctuations.

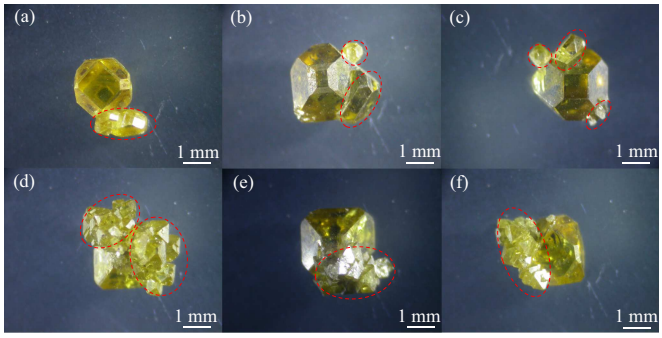


Fig. 2. Diamond crystals synthesized under different ambient temperature fluctuations (adjunct diamond). (a)–(c) Synthesized under temperature variation conditions. (d)–(f) Synthesized under significant temperature variation conditions.

3.2. Simulation results of catalyst temperature field

We set different temperatures for the bottom steel ring at various time intervals: specifically, 0 s–400 s at 50 °C, 400 s–800 s at 10 °C, 800 s–1000 s at 50 °C, 1000 s–1200 s at 20 °C, and 1200 s–1600 s at 50 °C. During the 400 s–800 s period, the temperature of the bottom steel ring drops sharply, simulating extremely cold external conditions. In the 800 s–1000 s period, the temperature of the bottom steel ring rises, simulating the return of external environmental temperatures to normal levels. From 1000 s–1200 s, the temperature of the bottom steel ring drops again, simulating another sudden decrease in external environmental temperatures. During the 1200 s–1600 s period, the temperature of the bottom steel ring rises once more, simulating the external environment's temperature returning to normal levels again. We aim to simulate fluctuations in external environmental temperatures, such as diurnal temperature variations, by changing the temperature of the lower steel ring, to analyze the impact of these fluctuations on the catalyst temperature.

To understand the influence of ambient temperature fluctuations on diamond crystal growth, we created a time history curve of catalyst temperature (0–1600 s). The results are shown in Fig. 3. Temperature fluctuations of the external environment have an important impact on the distribution of the temperature field inside the catalyst. Figure 3(a) shows the time history curve under environmental change, and Fig. 3(b) shows the local magnification of the time history curve under environmental change. When the environmental temperature changes, the catalyst temperature fluctuates accordingly. Figure 3(c) shows the time history curve in a constant environment, and Fig. 3(d) shows the local magnification of the time history curve in a constant environment. When the ambient temperature is constant, the catalyst temperature also remains unchanged. Through the curve, we can clearly observe the change trend and fluctuation range of catalyst temperature.

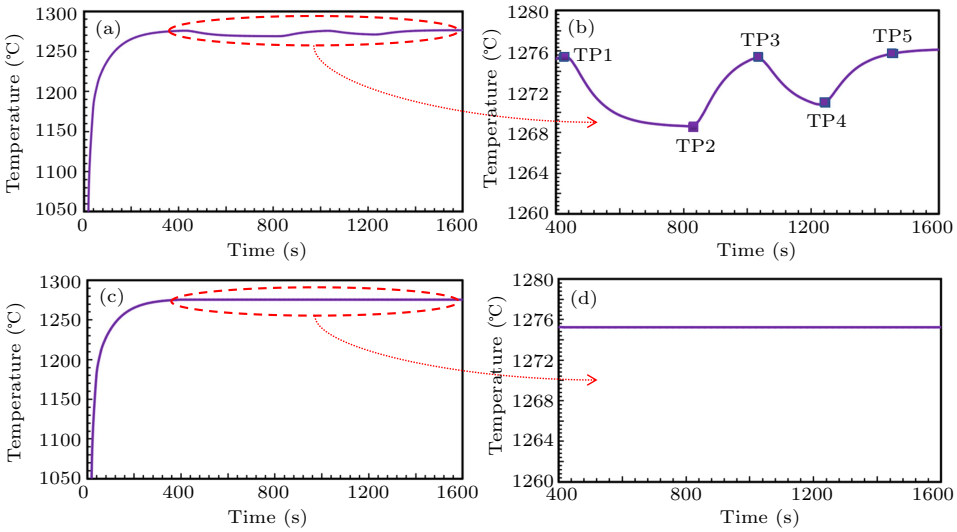


Fig. 3. (a) Time history curve under environmental change. (b) Local magnification of time history curve under environmental change. (c) Time history curve under constant environment. (d) Local magnification of time history curve under constant environment.

To further understand the effect of temperature change on diamond crystal growth, Figs. 4(a)–4(e) show the temperature distribution results for catalysts at 400 s, 800 s, 1000 s, 1200 s, and 1400 s, respectively. From the temperature distribution results, we can first observe that the temperature field is symmetrically distributed, with the high-temperature area in contact with the carbon source and the low-temperature area located around the seed position. Figures 4(a)–4(b) correspond to the process of environmental temperature decreasing from 400 s to 800 s. During this period, we can see that as the environmental temperature drops, the temperature of the catalyst also decreases, and the temperature at the crystal seed location decreases from 1275 °C to 1270 °C. Figures 4(b) and 4(c) correspond to the process of environmental temperature rising from 800 s to 1000 s. As the environmental temperature increases, the temperature of the catalyst also increases, and the temper-

ature at the crystal seed location rises to 1275 °C again. Figures 4(c) and 4(d) correspond to the process of environmental temperature decreasing again from 1000 s to 1200 s, and the temperature of the catalyst also decreases accordingly. The temperature at the crystal seed location decreases to 1271 °C. Finally, Figs. 4(d) and 4(e) correspond to the process of environmental temperature rising again from 1200 s to 1400 s, and the temperature of the catalyst also rises accordingly. The temperature at the crystal seed location rises to 1275 °C once again. The numerical results indicate that changes in the external environmental temperature directly cause fluctuations in the temperature field within the synthesis assembly, with the temperature at the seed and carbon source sites decreasing as the external environmental temperature drops.

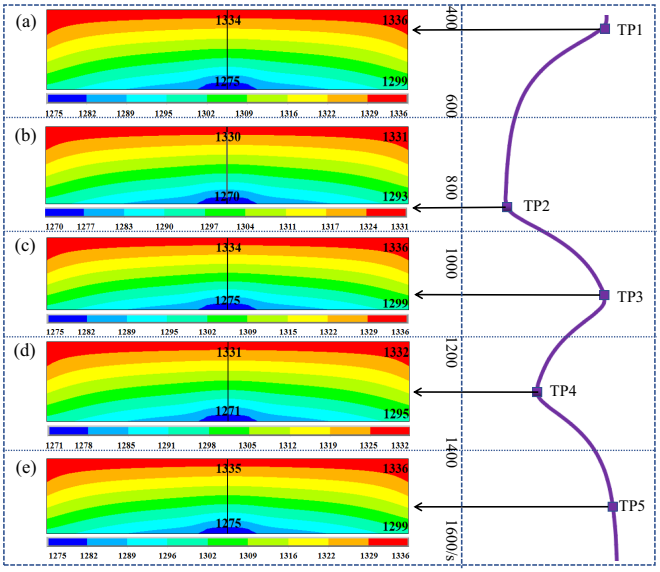


Fig. 4. Catalyst temperature fields corresponding to (a) TP1, (b) TP2, (c) TP3, (d) TP4, and (e) TP5.

3.3. Theoretical explanation of the adjunct diamond growth

According to the solvent theory of diamond growth, under a certain temperature gradient, the solubility of diamond in the molten catalyst is greater in the high-temperature region than in the low-temperature region. The supersaturated solubility generated in the high-temperature region compared to that in the low-temperature region is the direct driving force for the crystallization of diamond.[33–35] Based on the research results concerning the catalyst temperature field distribution and the time history curve under environmental changes, we have deeply explored the impact of environmental temperature fluctuations on the growth of diamond crystals. The temperature changes within the catalyst directly determine the solubility of carbon in the catalyst. This implies that any alteration in the catalyst's internal temperature field will lead to a corresponding change in the solubility of carbon in the metal catalyst. As the synthesis time progresses, with the synthesis pressure held constant, fluctuations in the catalyst temperature cause changes in the local temperature within the nucleation zone. Such temperature variations create favorable conditions for nucleation at multiple excitation points on the crystal surface. Consequently, the secondary nucleation of diamond occurs during the growth process, resulting in the phenomenon of intercrystalline growth. The adjunct diamond growth diagram is as shown in Fig. 5.

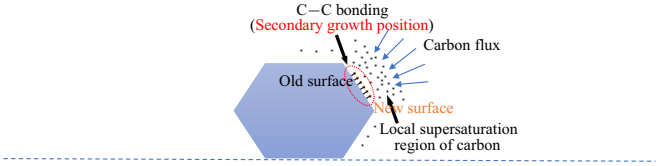


Fig. 5. Adjunct diamond growth diagram.

4. Conclusions

In this study, ambient temperature fluctuations were simulated by altering the boundary conditions, specifically by changing the temperature of the steel ring at various times to mimic the external environmental temperature fluctuations during the corresponding periods. The temperature field within the catalyst was simulated using the finite element method. Based on the simulation and experimental results, we can conclude the following: external environmental temperature fluctuations cause similar fluctuations within the catalyst, which in turn lead to changes in the catalyst's solubility. These solubility changes make the crystal surface prone to secondary crystallization, resulting in adjunct crystal formation. This research has uncovered the impact of temperature field changes in the catalyst on the solubility of carbon in metal catalysts and the growth process of diamonds. It provides a theoretical foundation for a deeper understanding of the critical role of the catalyst temperature field in the material synthesis process and holds significant guiding value for practical production applications. Building on these findings, future research can delve into additional influencing factors and the behavior of the catalyst temperature field under synthetic conditions, aiming to offer more scientific guidance for optimizing the material synthesis process.

Acknowledgements

This project was supported by the Natural Science Foundation of Chongqing, China (Grant Nos. CSTB2023NSCQ-MSX0362 and CSTB2023NSCQ-LZX0100), the Science and Technology Research Program of Chongqing Municipal Education Commission (Grant No. KJZD-K202401403), the Scientific Research Project of the Science and Technology Bureau of Fuling (Grant No. FLKJ2025AAG2003), and the Henan Provincial Natural Science Foundation (Grant No. 252300421475).

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