Numerical optimization of the thermal field in Bridgman detached growth

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The global modeling of the thermal field in two vertical Bridgman-like crystal growth configurations, has been performed to get optimal thermal conditions for a successful detached growth of Ge and CdTe crystals. These computations are performed using the CrysMAS code and expand upon our previous analysis [1] that propose a new mechanism involving the thermal field and meniscus position to explain stable conditions for dewetted Bridgman growth.

The analysis of the vertical Bridgman configuration with two heaters, used by Palosz et al.[2] for the detached growth of Ge, shows, consistent with their results, that the large wetting angle of germanium on boron nitride surfaces was an important factor to promote a successful detached growth. Our computations predict that by initiating growth much higher into the hot zone of the furnace, the thermal conditions will be favorable for continued detachment even for systems that did not exhibit high contact angles.

The computations performed for a vertical gradient freeze configuration with three heaters representative of that used for the detached growth of CdTe [3,4], show favorable thermal conditions for dewetting during the entirely growth run described in [3]. Improved thermal conditions are also predicted for coated silica crucibles when the solid-liquid interface advances higher into the hot zone during the solidification process.

The second set of experiments on CdTe growth described in [4] has shown the reattachment of the crystal to the crucible after few centimeters of dewetted growth. The thermal modeling of this configuration shows a second solidification front appearing at the top of the sample and approaching the middle line across the third heater. In these conditions, the crystal grows detached from the bottom, but will be attached to the crucible in the upper part because of the solidification without gap in this region. The solidification with two interfaces can be avoided when the top of the sample is positioned below the middle position of the third furnace.

References

[1] C. Stelian, A. Yeckel, J.J. Derby, Influence of thermal phenomena on crystal reattachment during the dewetted Bridgman growth, J. Crystal Growth, in press.
[2] W. Palosz, M. P. Voltz, S. Cobb, S. Motakef, F. R. Szofran, J. Crystal Growth, 277 (2005) 124.
[3] N. Chevalier, P. Dusserre, J.P. Garandet and T. Duffar, J. Crystal Growth, 261 (2004) 590.
[4] M. Fiederle et al., J. Crystal Growth, 267, 2004, 429.

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Project Description

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References
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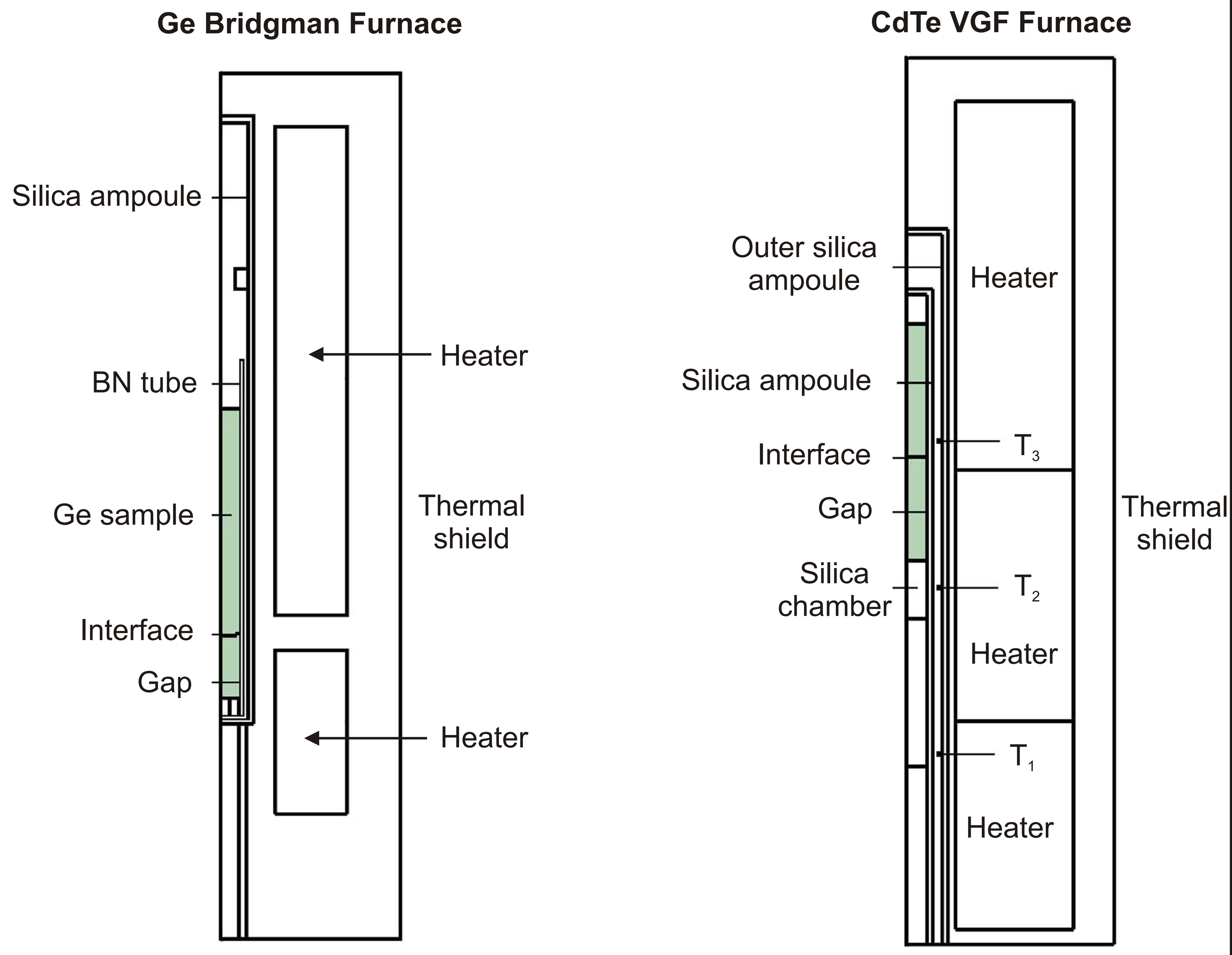
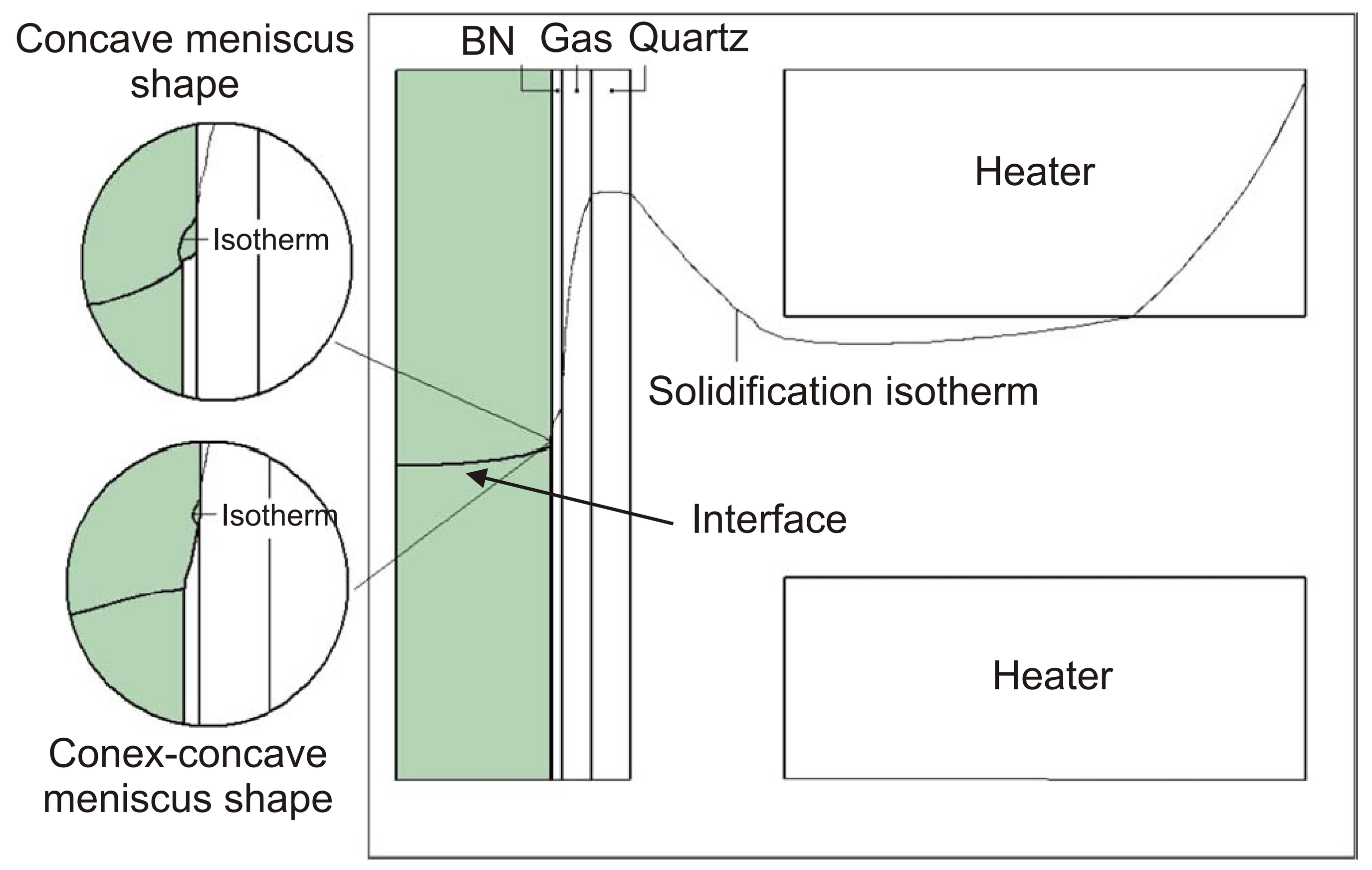
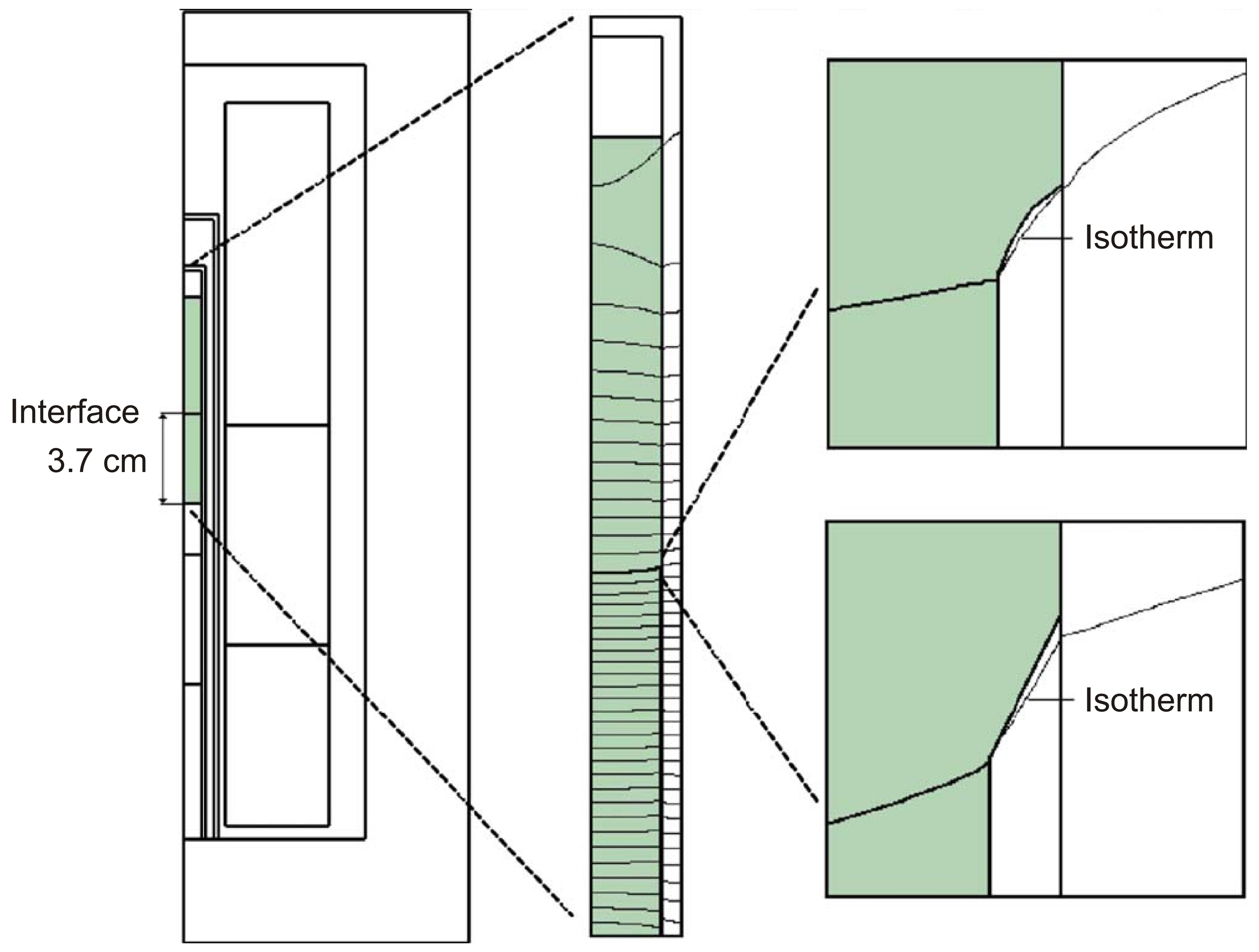


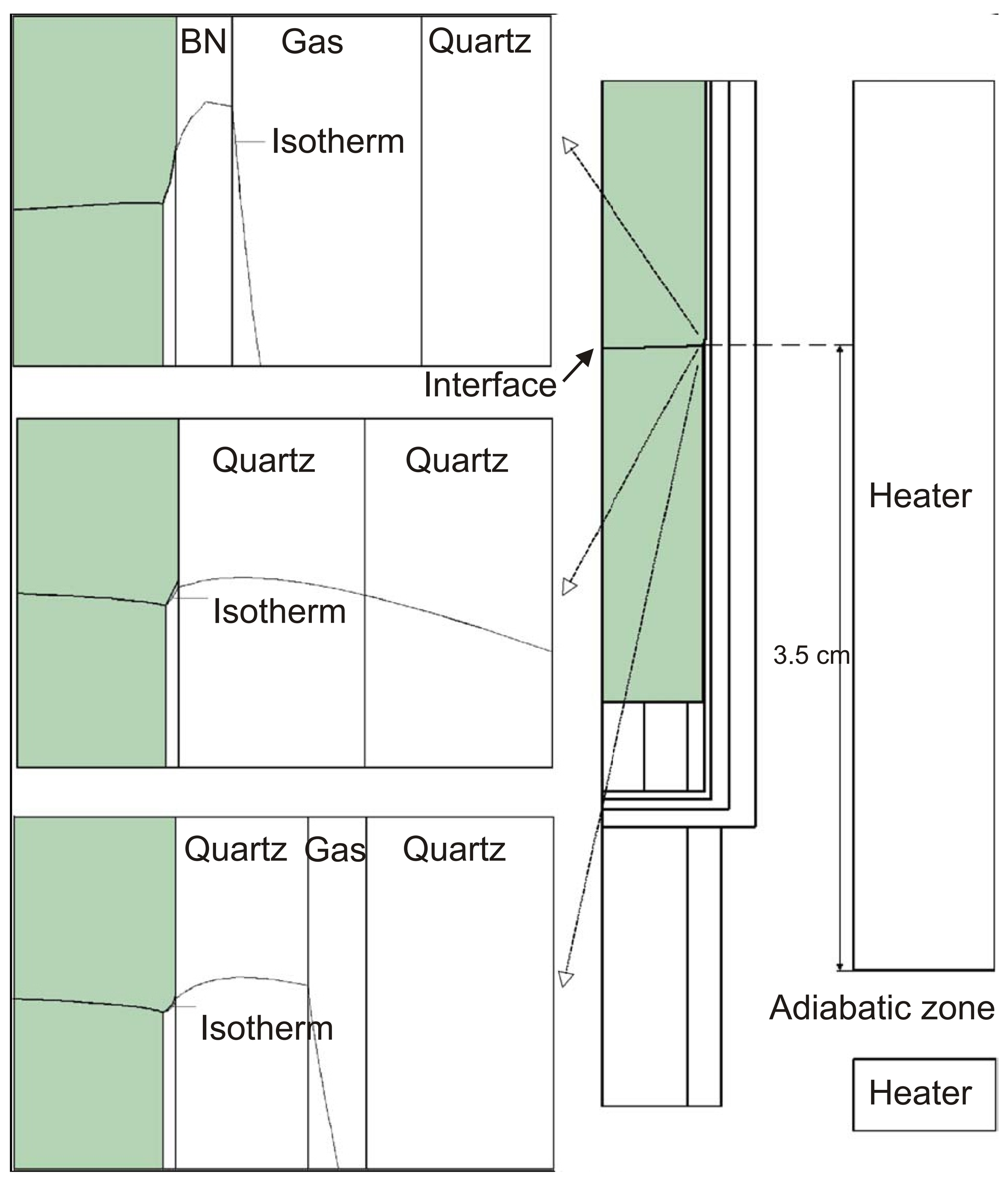
Schematic diagrams of the computational domains for the Bridgman configuration with two heaters employed by Palosz et al. [2] and the VGF configuration with three heaters employed by Chevalier et al. [3].



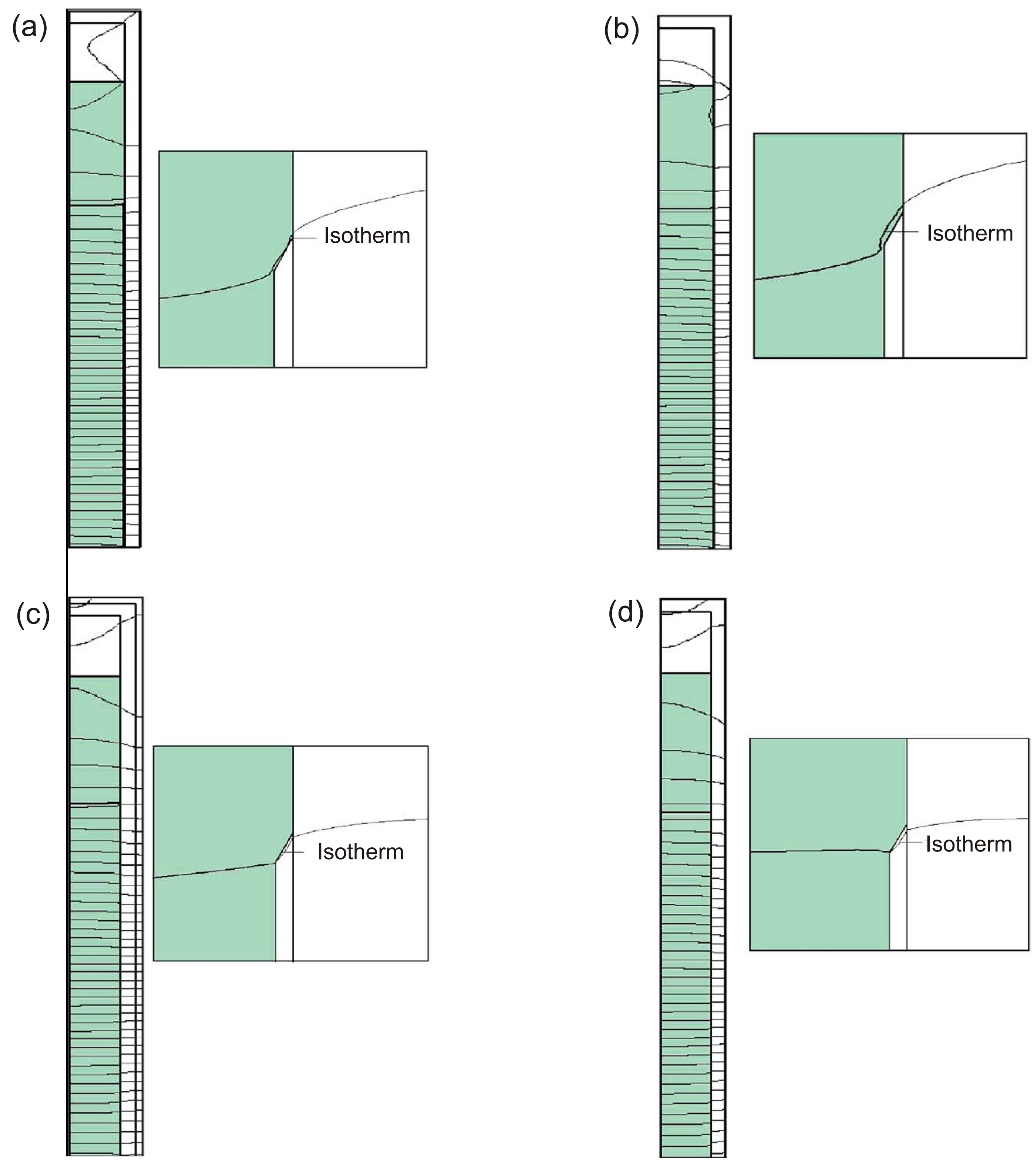
Relative positions of the solidification isotherm and meniscus predicted for the configuration using a BN inner tube: the position of the solid-liquid interface is located in the center of the adiabatic zone. Two detailed views show cases for a convex-concave meniscus (below) and a concave meniscus (above).



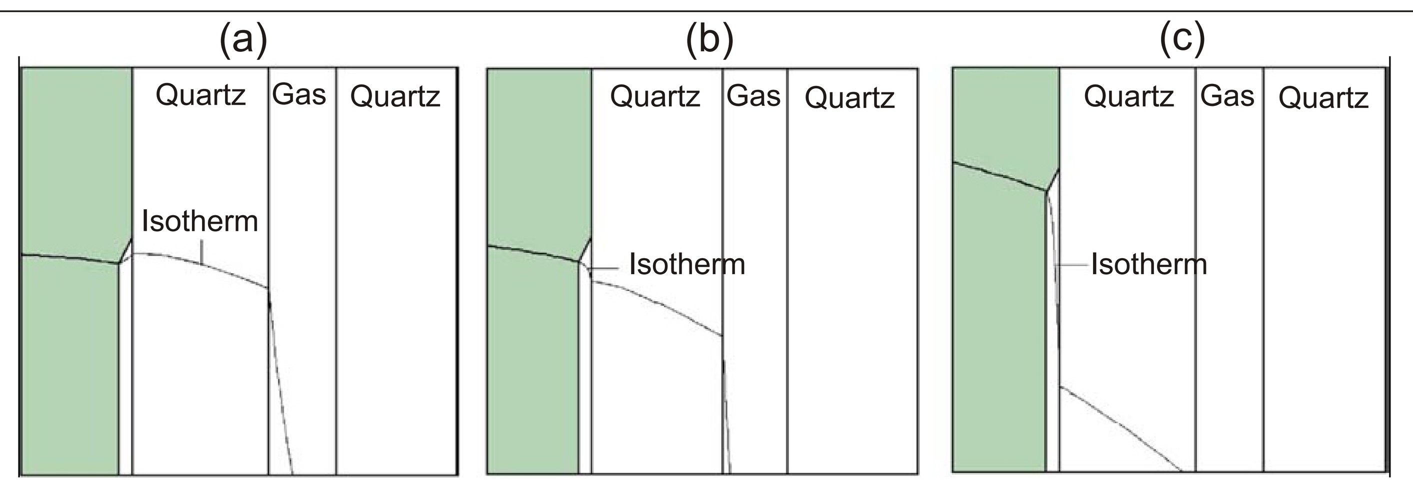
Thermal field predicted for the initial configuration of successful detached growth described in [3]. Two detailed views show relative positions of the solidification isotherm and meniscus for a curved meniscus (above) and a straight-line approximation to the meniscus (below).



Relative positions of the solidification isotherm and meniscus predicted for several different ampoule-crucible configurations; the interface is positioned at 3.5 cm above the adiabatic zone.



Thermal field predicted for an advanced position of the interface, corresponding to 5.9 cm length of the solid. Detailed views show relative positions of the solidification isotherm and meniscus. Case for (a) semitransparent quartz ampoule; (b) completely transparent quartz ampoule; (c) semitransparent quartz ampoule with its exterior coated by a graphite layer; and (d) opaque quartz ampoule.



Evolution of the position of the solidification isotherm when the furnace is translated up to simulate growth; the ampoule configuration consists of two quartz tubes separated by gas: (a) initial state; (b) heaters translated by 2 cm; and (c) heaters translated by 3 cm.