

NIST 2003 Workshop

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On the formation of a β layer in $\gamma + \beta$ diffusion couples and diffusion paths with “horns”

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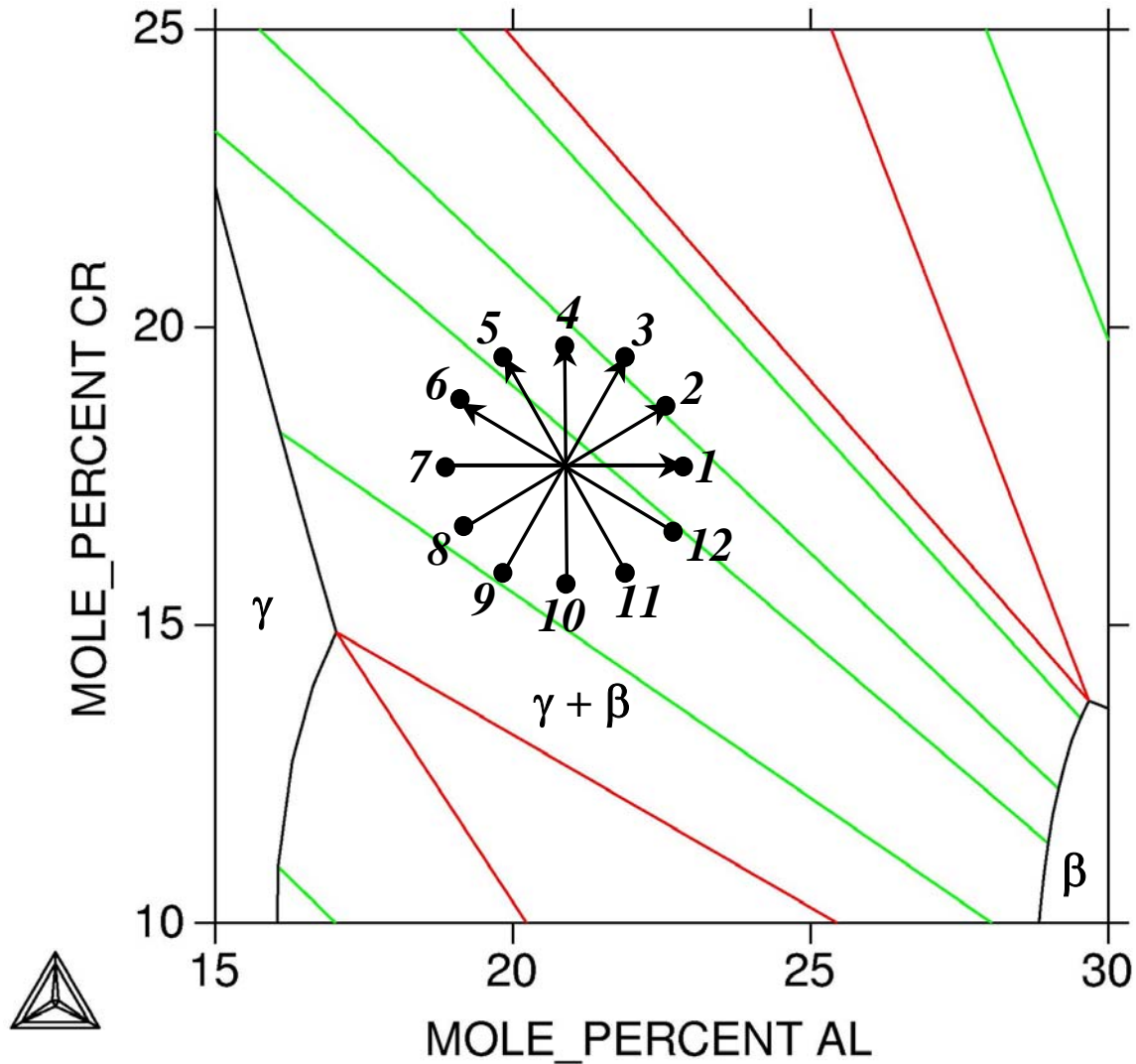


Outline

- **The experimental observation of a β layer in certain $\gamma + \beta$ diffusion couples**
- **Zigzag diffusion paths and the diffusion paths with “horn”**
- **The characterization of “horn”**
- **The transition between inward and outward “horns”**
- **The explanation of the β layer formation**



β layer in $\gamma + \beta$ diffusion couples



β layer in $\gamma + \beta$ diffusion couples

β layer formed

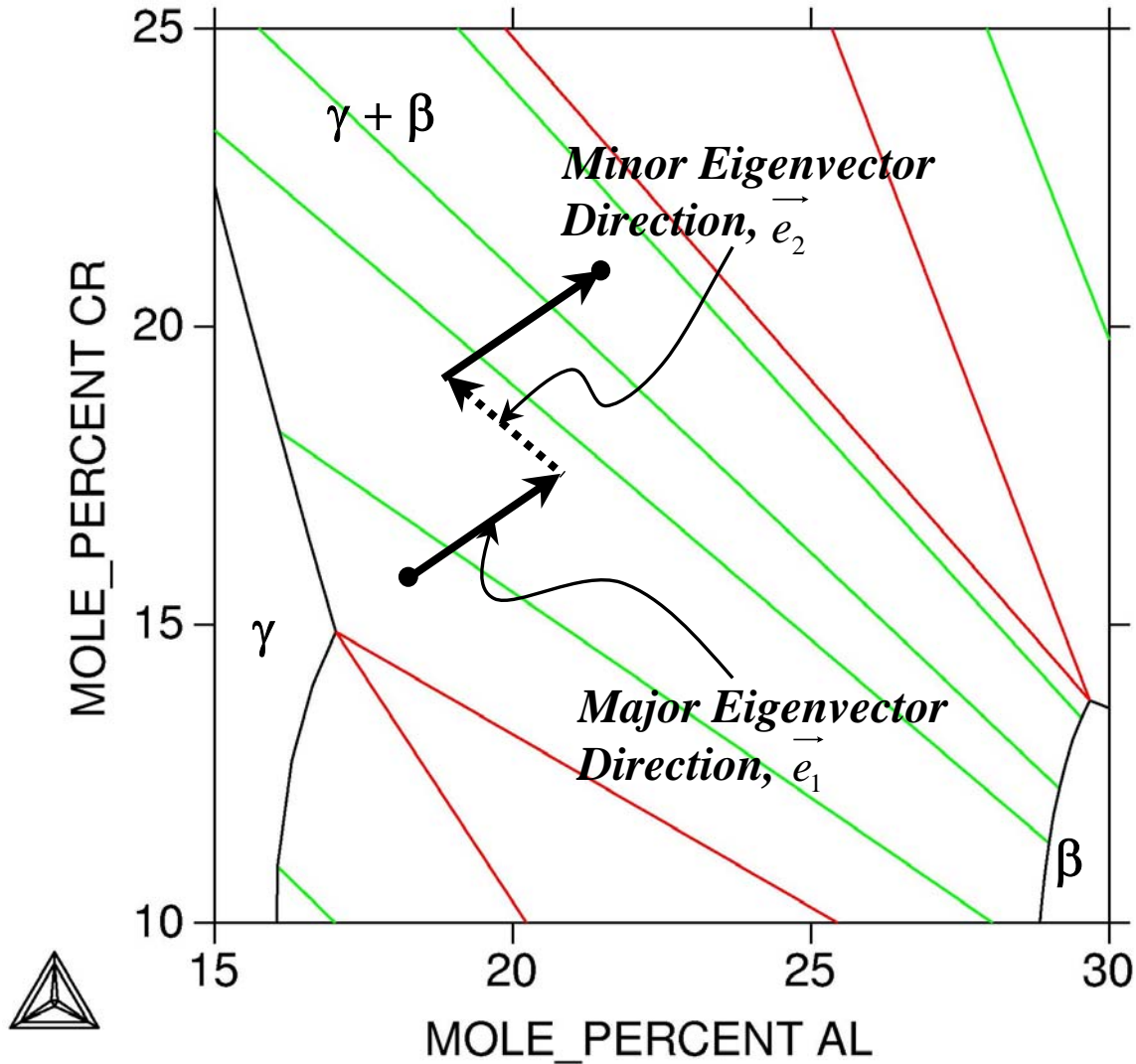
NO β layer formed

$\gamma + \beta < \beta > \gamma + \beta$

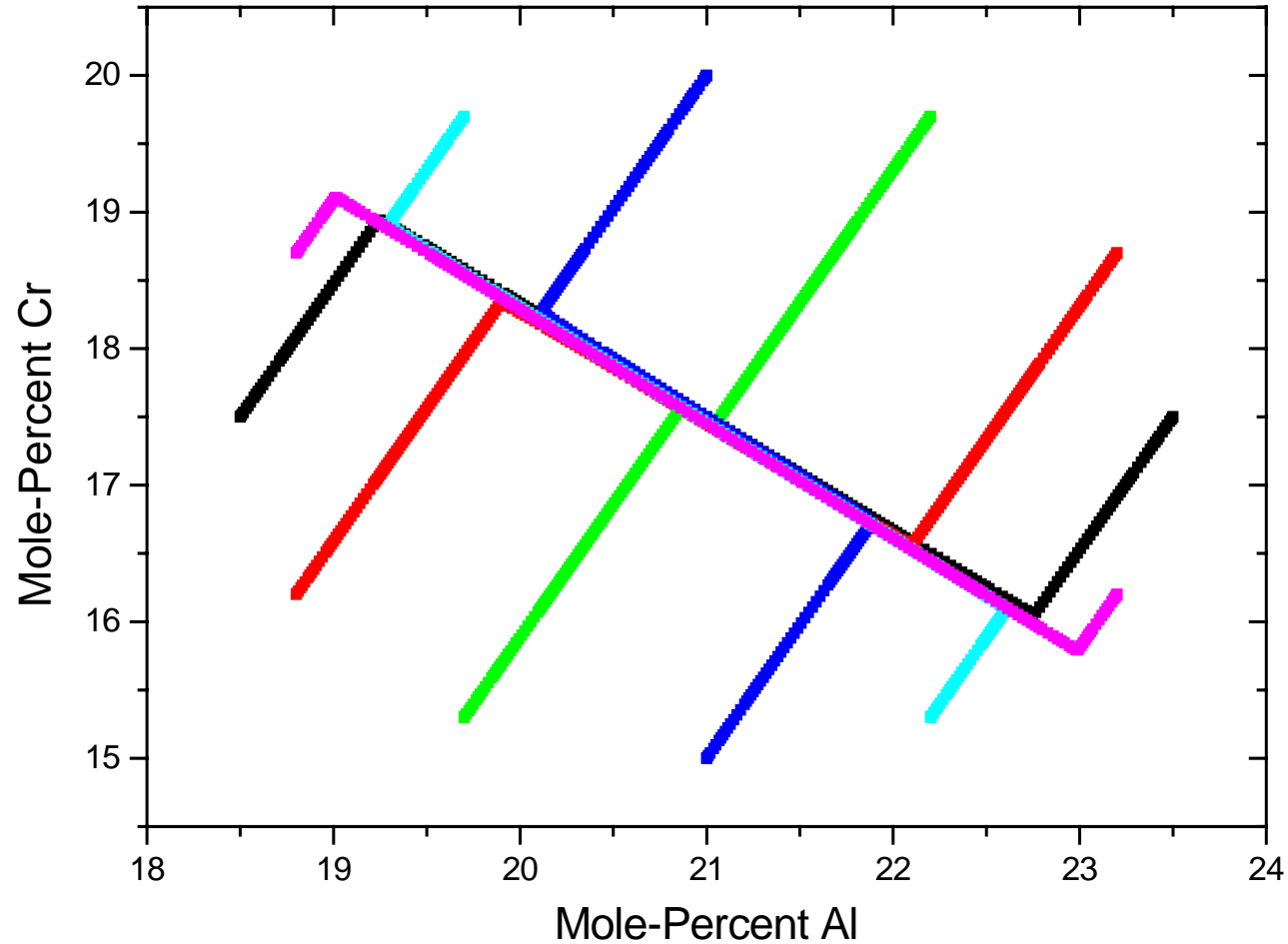
$\gamma + \beta / \gamma + \beta$



Error function prediction

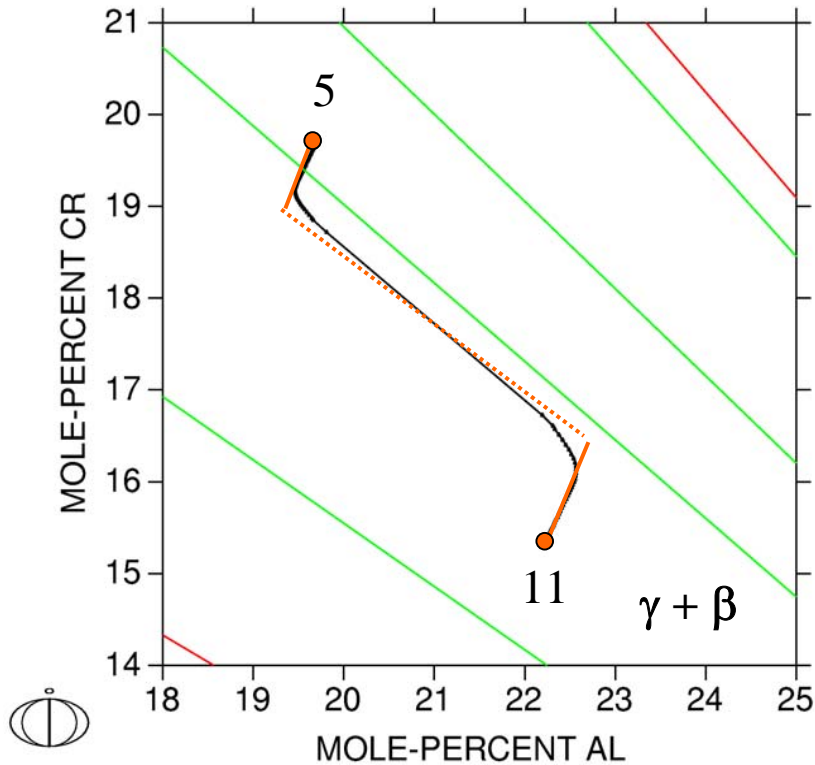


Zigzag diffusion paths of $\gamma + \beta$ couples

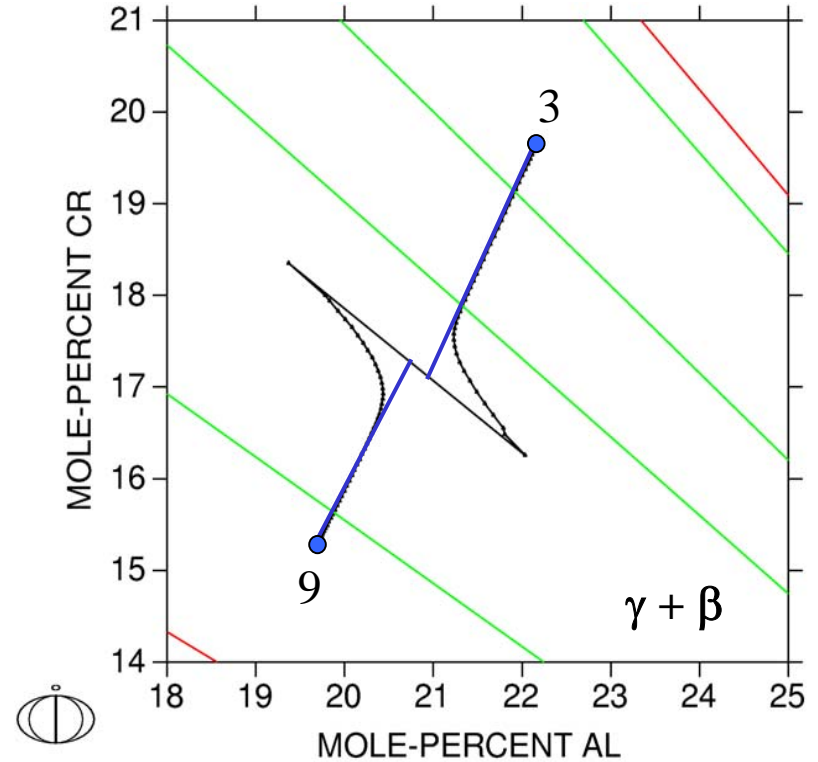


Diffusion paths with “horns”

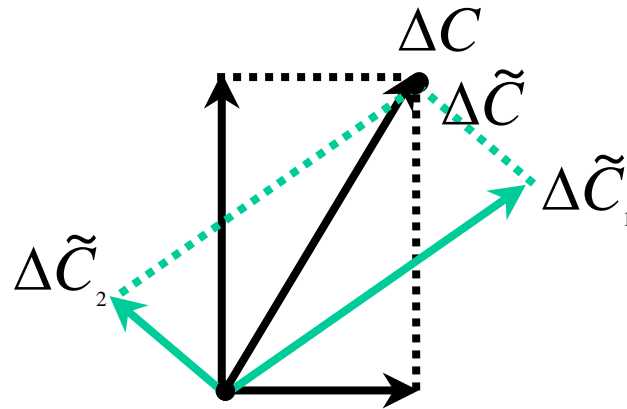
Horns Point Inward



Horns Point Outward

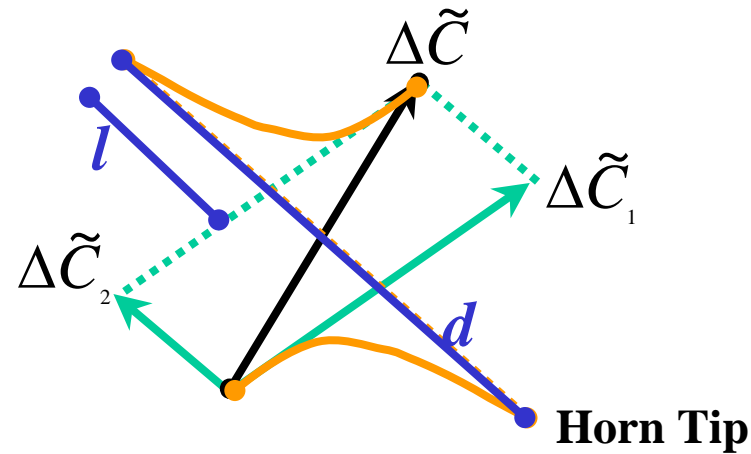


Characterization of ‘horns’



$$\begin{aligned} [\tilde{D}^{eff}] &= [\alpha][D^{eff}][\alpha^{-1}] & \begin{pmatrix} \Delta\tilde{C}_1 \\ \Delta\tilde{C}_2 \end{pmatrix} &= \begin{bmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{bmatrix} \begin{pmatrix} \Delta C_1 \\ \Delta C_2 \end{pmatrix} \\ [\Delta\tilde{C}] &= [\alpha][\Delta C] \end{aligned}$$

Characterization of “horns”



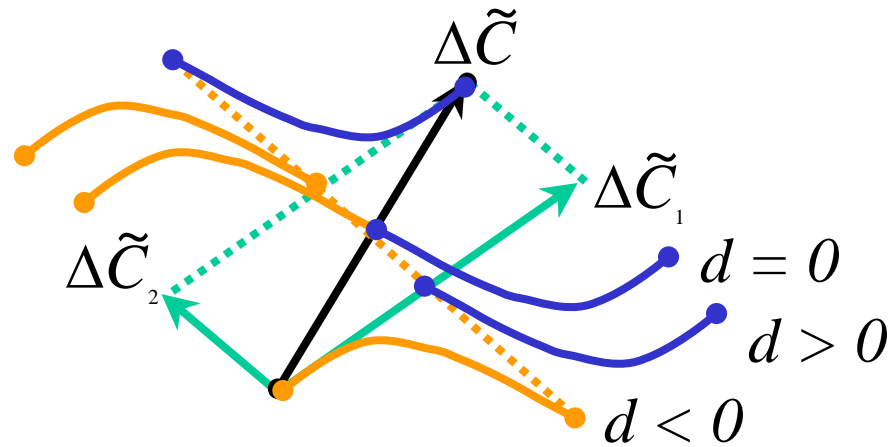
$$2l = \left| \Delta\tilde{C}_2 - d(\Delta\tilde{C}_1, \Delta\tilde{C}_2) \right|$$

d = The distance between horn tips

l = The horn length

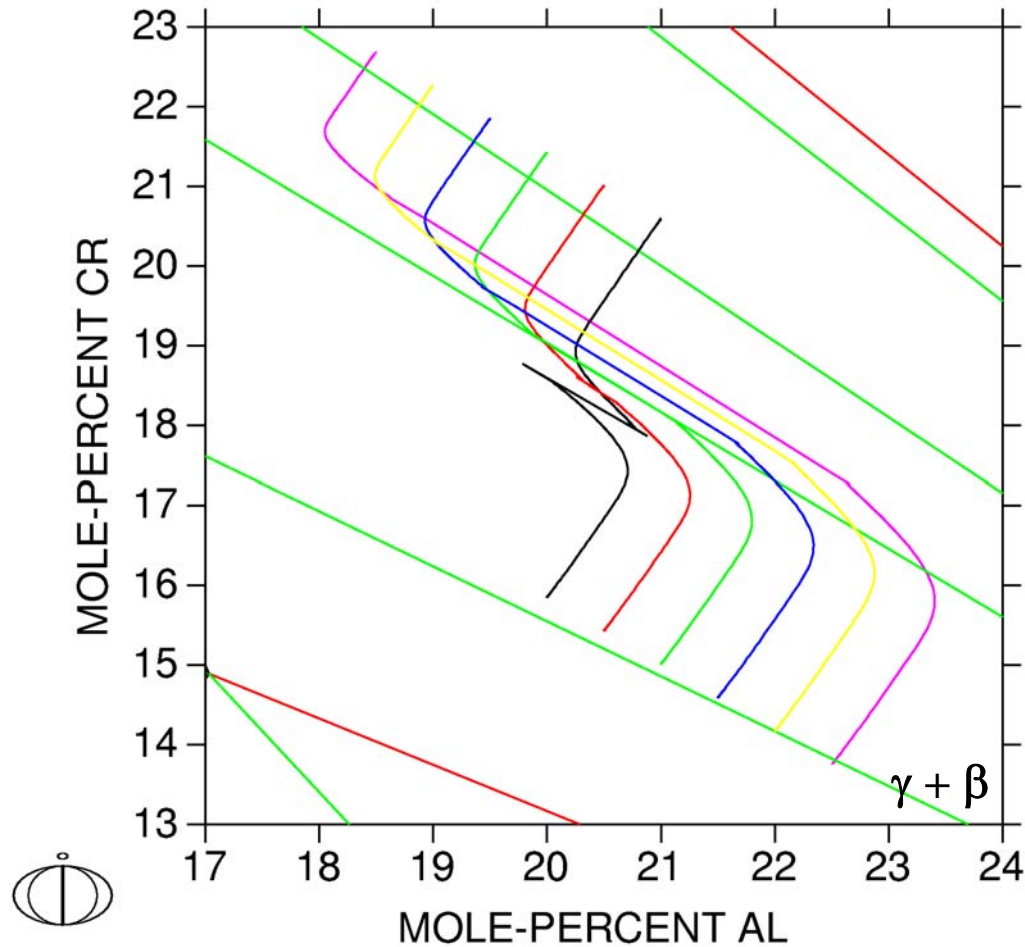


Characterization of “horns”

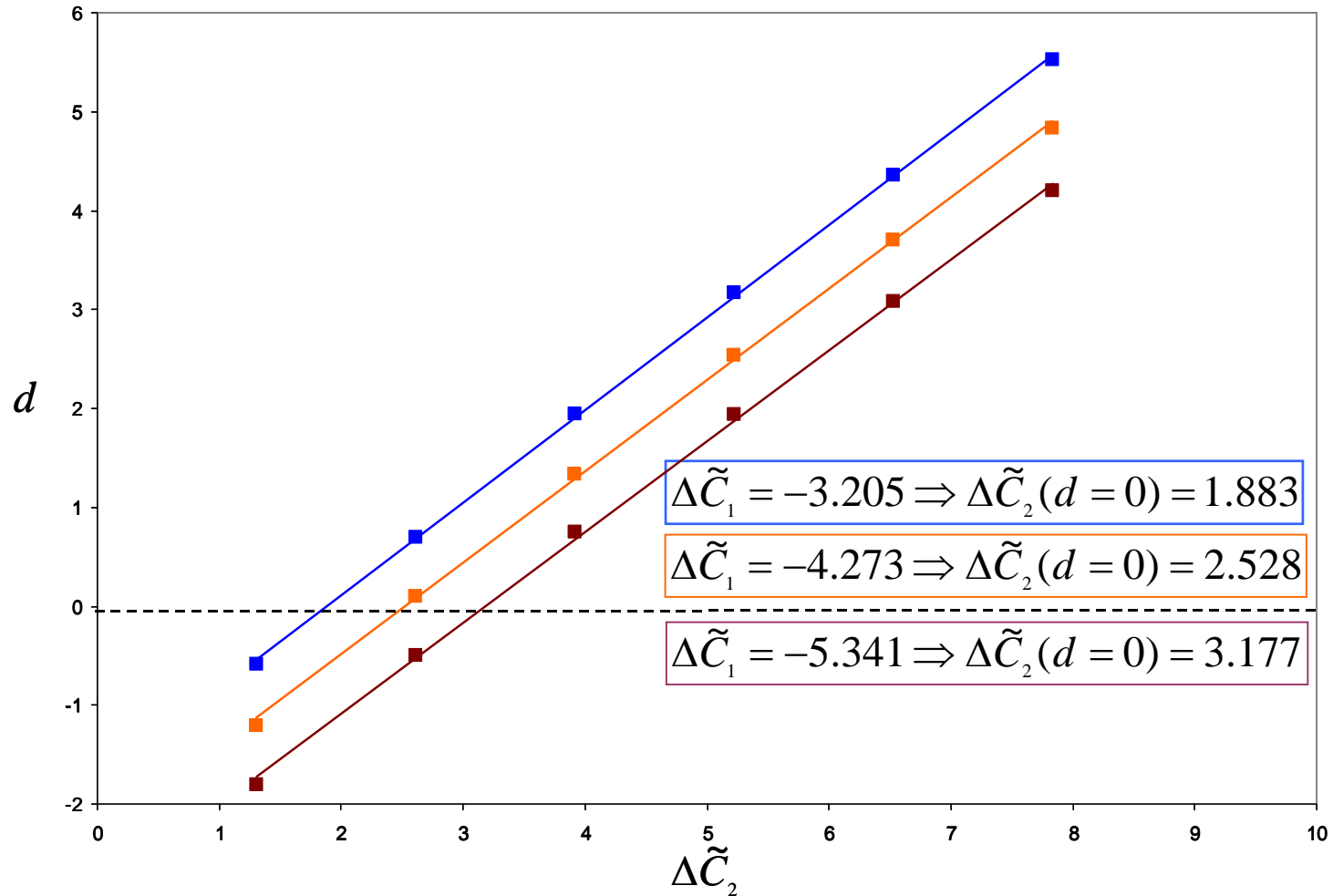


“Horn” change with compositions

$$\Delta \tilde{C}_1 = -4.27$$

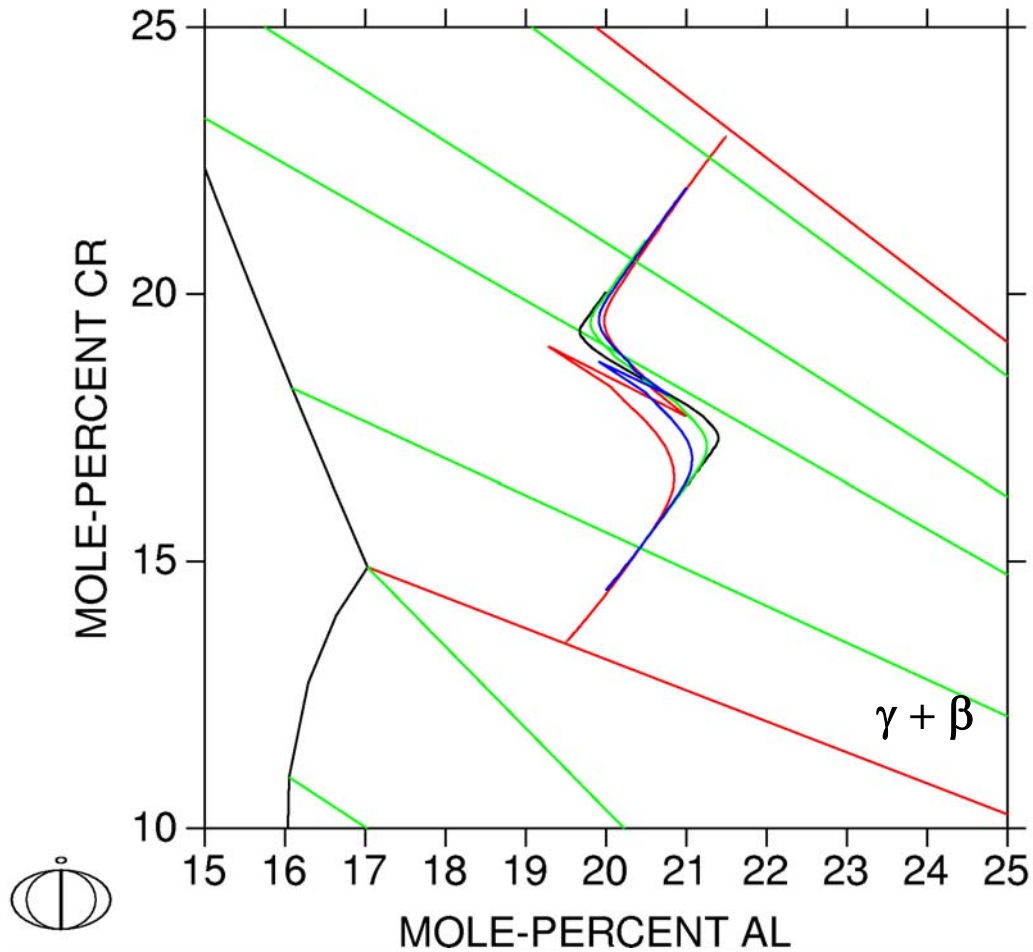


“Horn” change with compositions

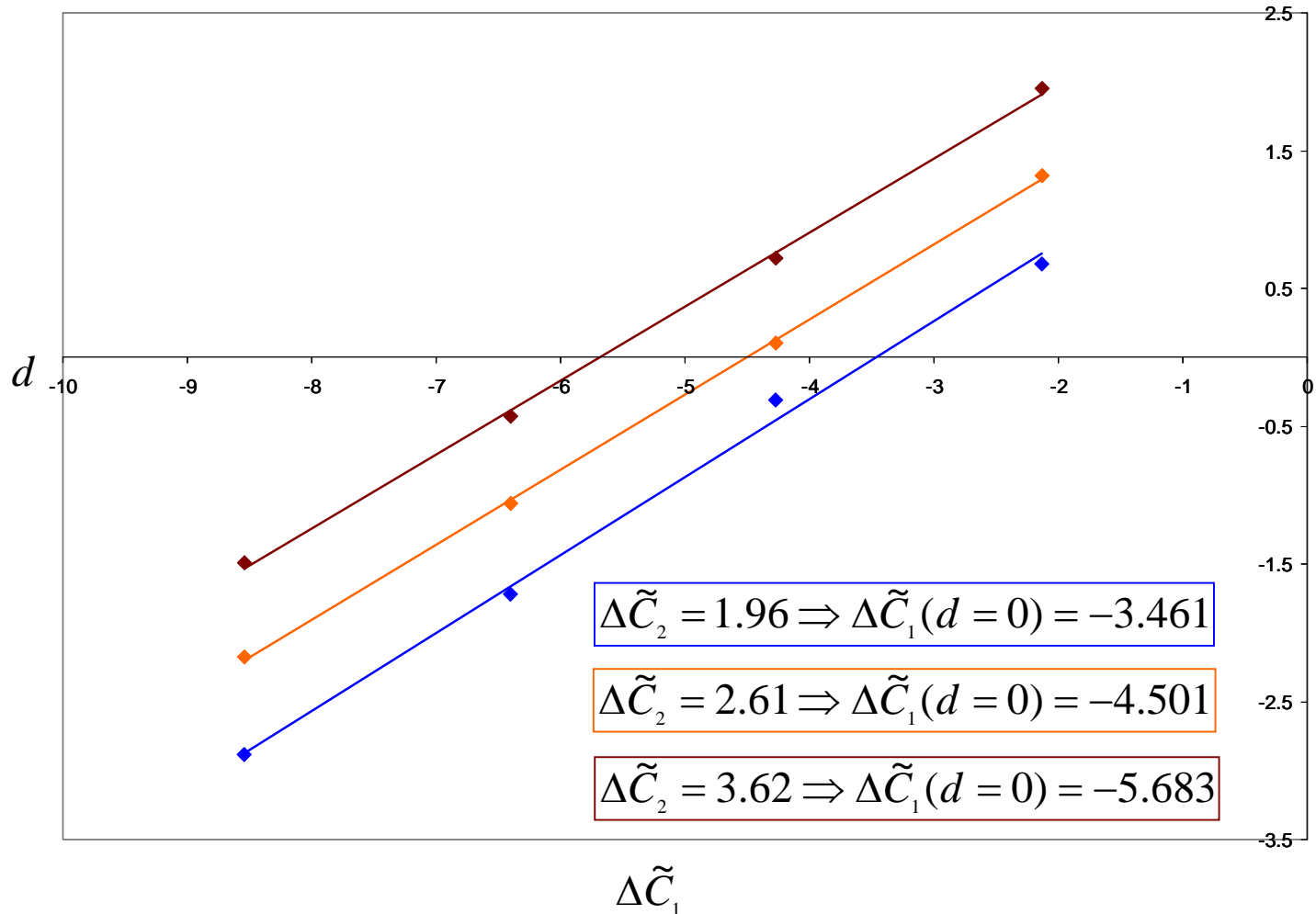


“Horn” change with compositions

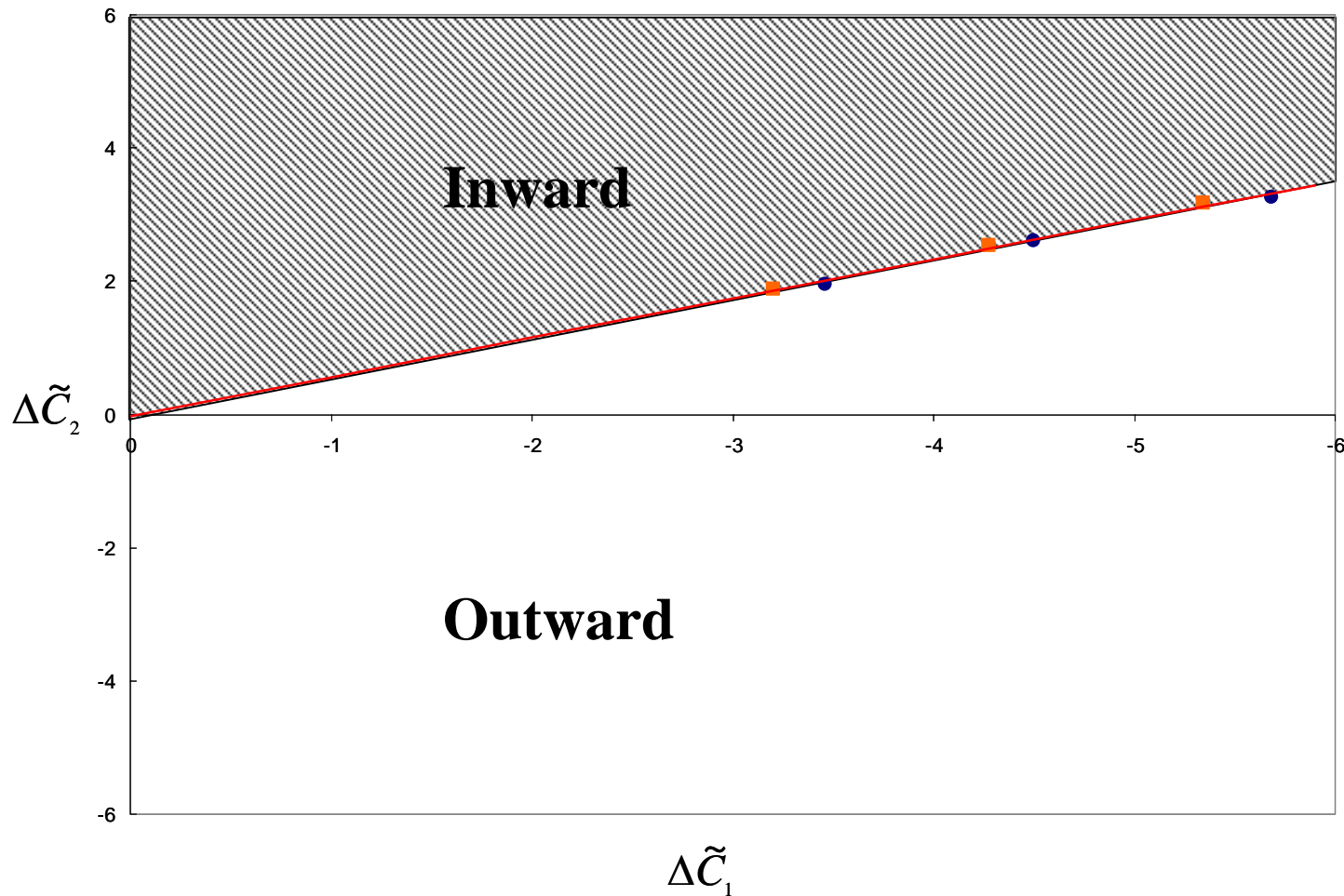
$$\Delta \tilde{C}_2 = -2.61$$



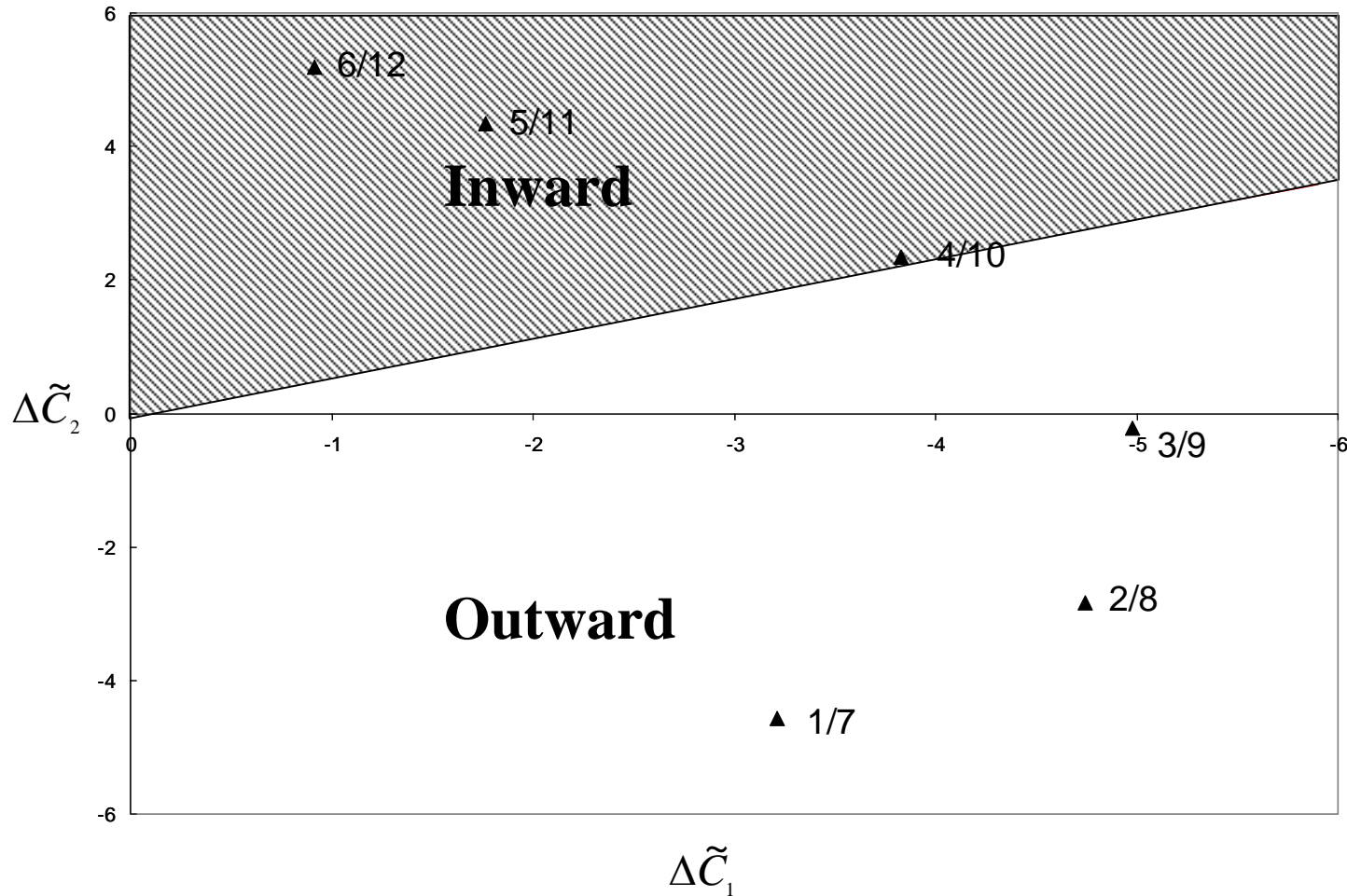
“Horn” change with compositions



Transition between inward and outward horns



The formation of β layer



Summary

- **DICTRA simulations of $\gamma+\beta$ diffusion couples show sharp deviations from linear zigzag paths, appearing as inward or outward pointing horns.**
- **The transition between inward and outward “horns” is related to the change in composition.**
- **The formation of a β layer in experimental $\gamma + \beta$ diffusion couples is associated with predicted diffusion paths containing outward horns.**

