TMS 2005 Meeting

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Prediction and Characterization of Diffusion Paths with "Horns" in Two-Phase Ternary Diffusion Couples

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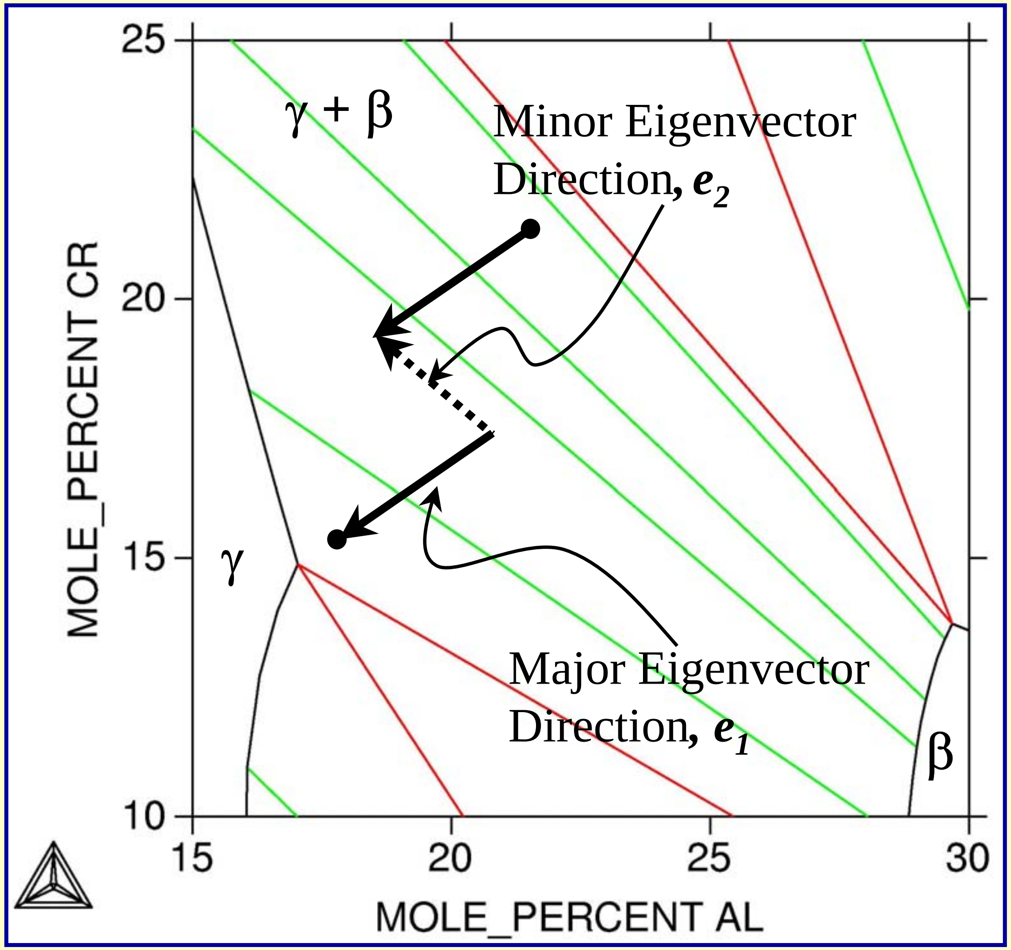
Outline

- Linear “zigzag” diffusion paths
- Non-linear diffusion paths with “horns”
- Characterization of “horns”
- Prediction of the type of “horns”
- Variation of “horns” with composition
- Summary

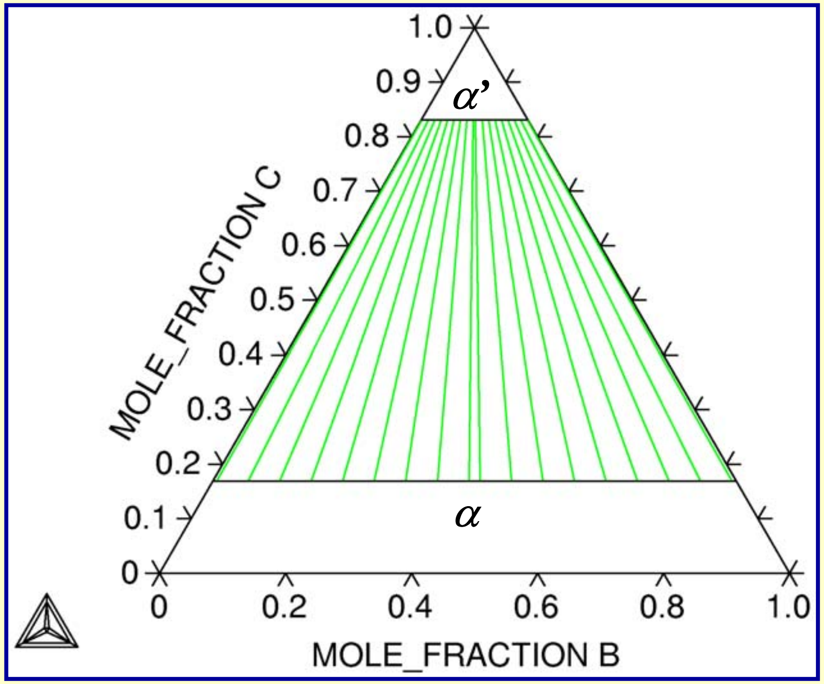
Zigzag Diffusion Paths

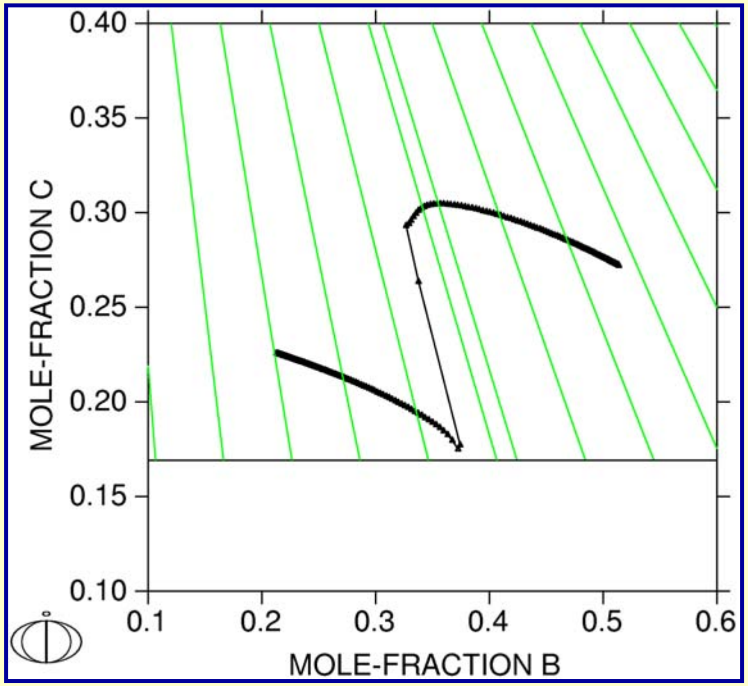


$$[D^{eff}] = [D^{\gamma}] \cdot [C^{TM}]$$

Diffusion Paths from DICTRA Simulation

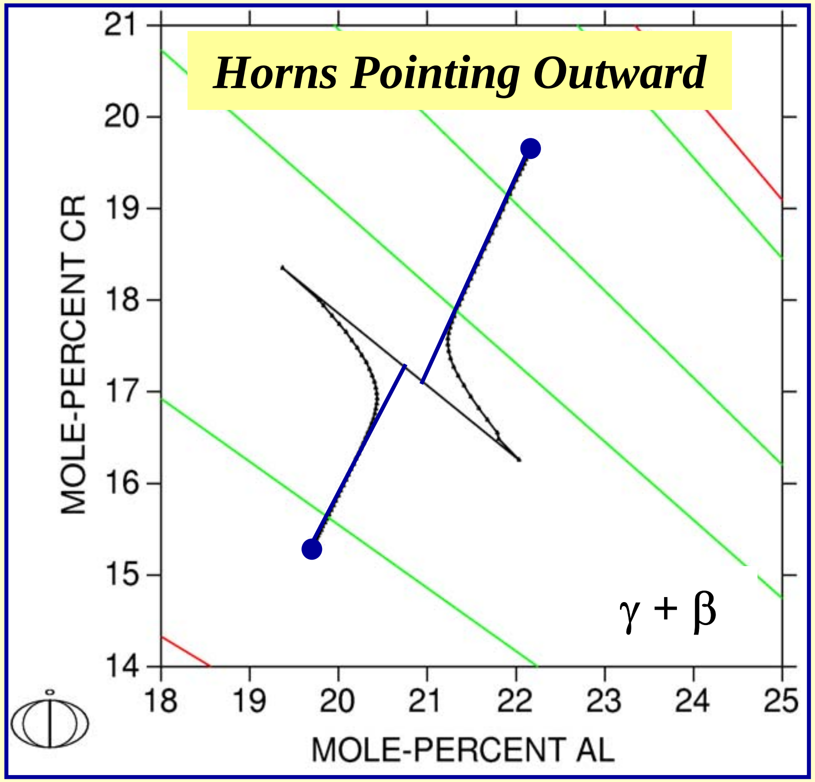
Single-horns in $\alpha + \alpha'$ two-phase A-B-C diffusion couples

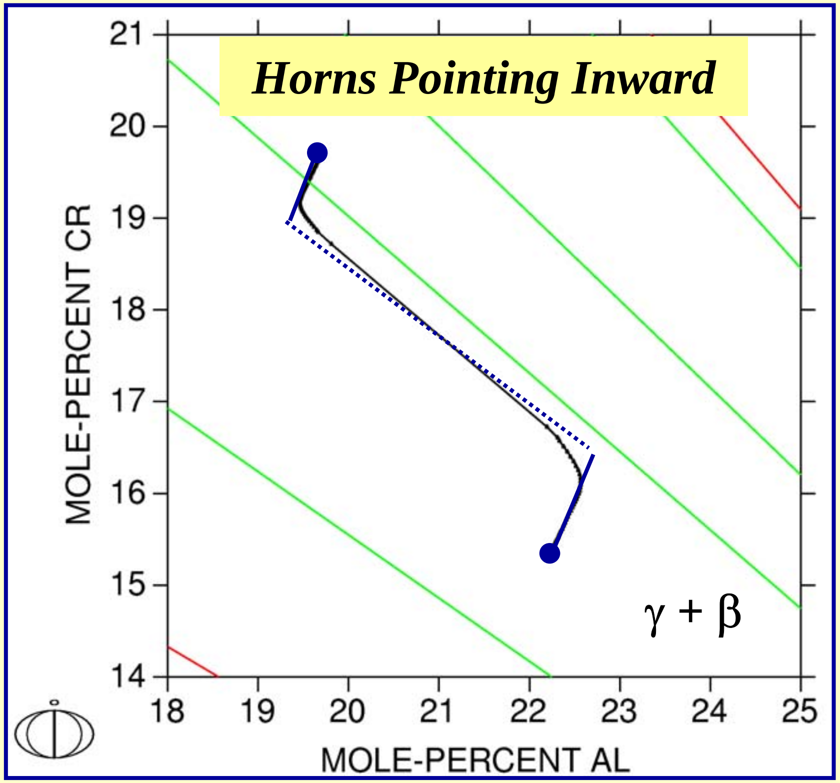




Diffusion Paths from DICTRA Simulation

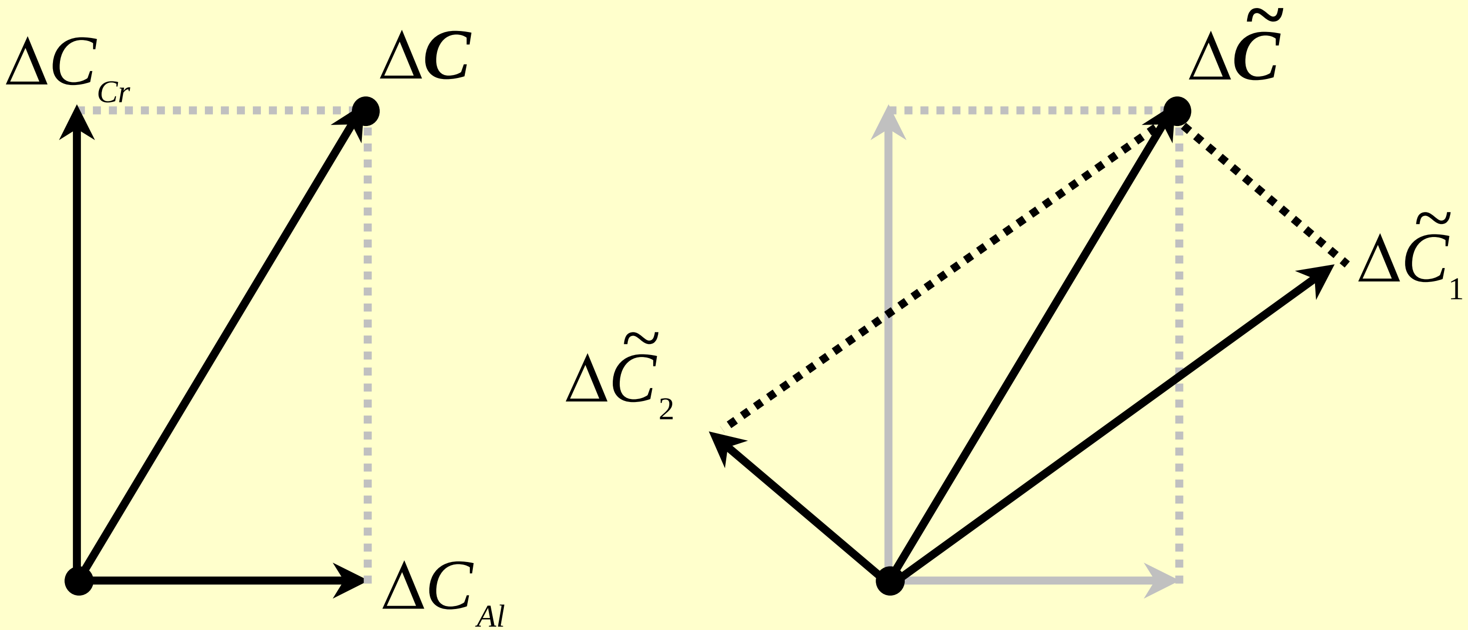
Double-horn in $\gamma + \beta$ two-phase Ni-Cr-Al diffusion couples





Characterization of "Horns"

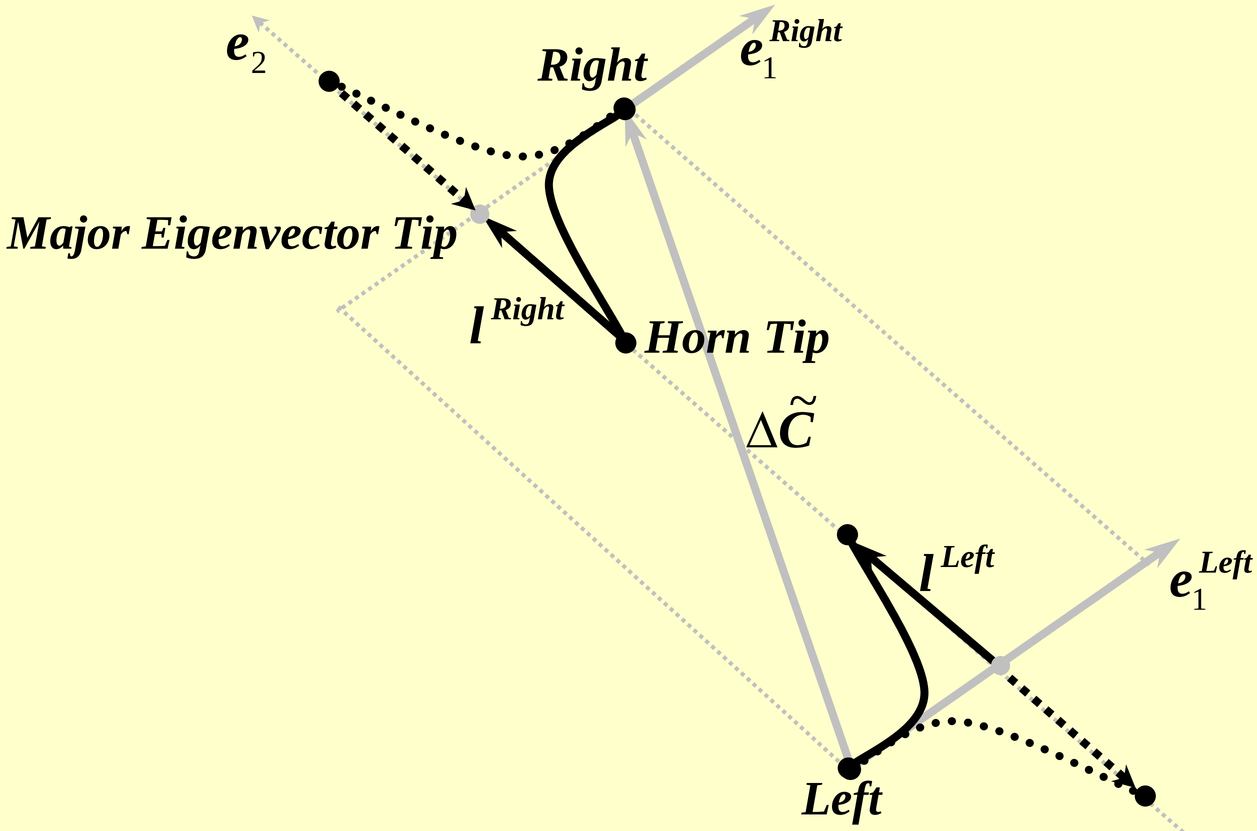
Transformation of coordinates



$$\boxed{[\Delta \tilde{C}) = [\alpha][\Delta C)}$$

Characterization of “Horns”

Correlation of the type of horns with the horn length

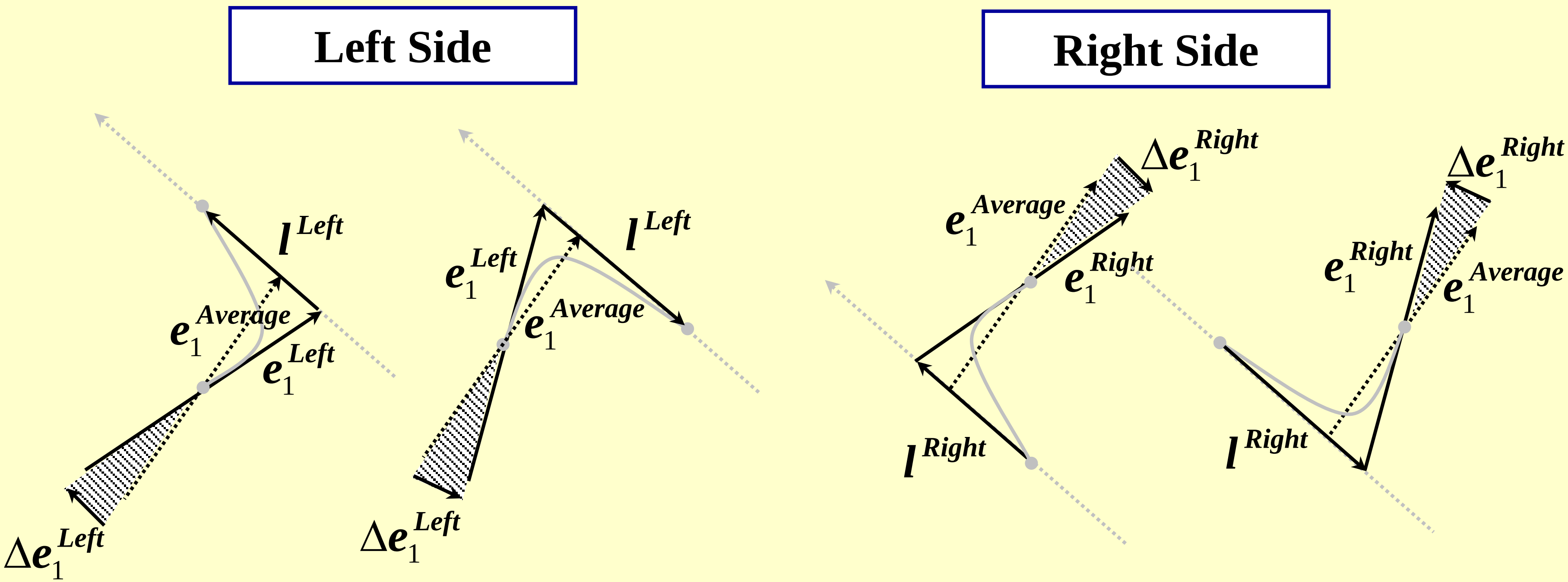


Double-horn: l^{Right} and l^{Left} have the same sign

Single-horn: l^{Right} and l^{Left} have the opposite sign

Prediction of the Type of Horns

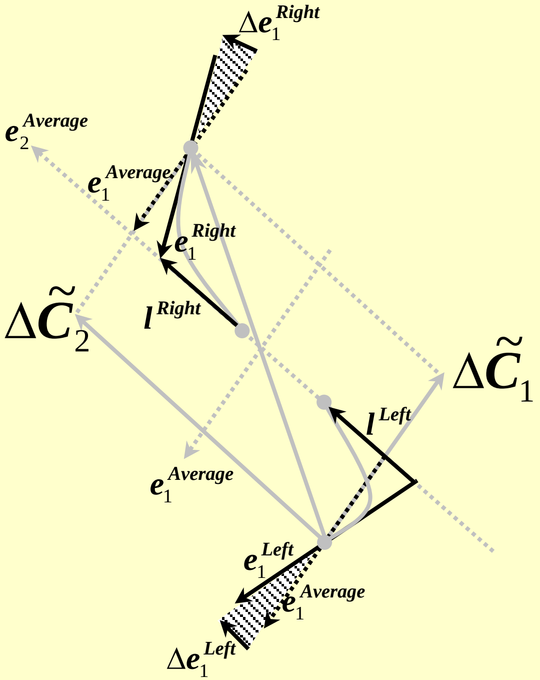
The relative position of two major eigenvectors



Prediction of the Type of Horns

The relative position of two major eigenvectors

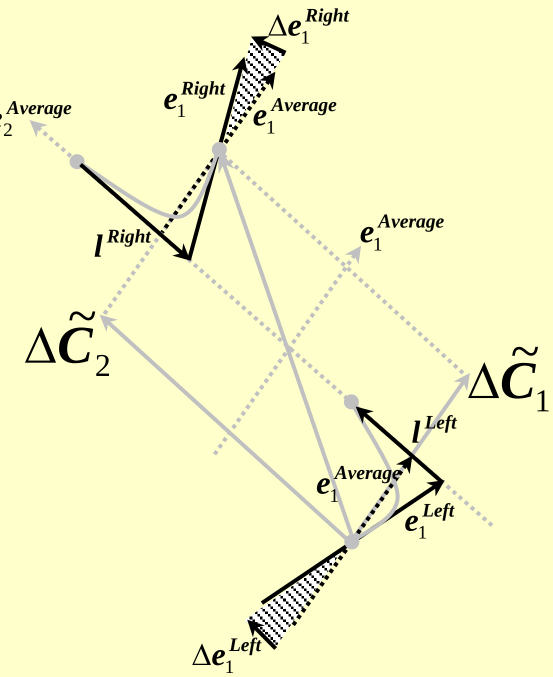
Double-horn



If $\Delta e_1^{Left} > 0$, then $l^{Left} \cdot \Delta\tilde{C}_2 < 0$

If $\Delta e_1^{Left} < 0$, then $l^{Left} \cdot \Delta\tilde{C}_2 > 0$

Single-horn

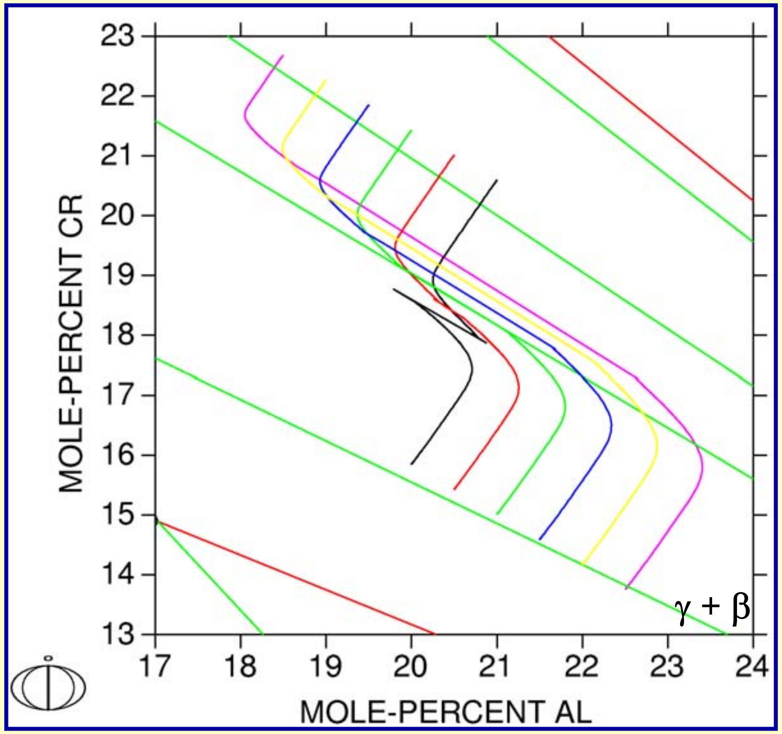


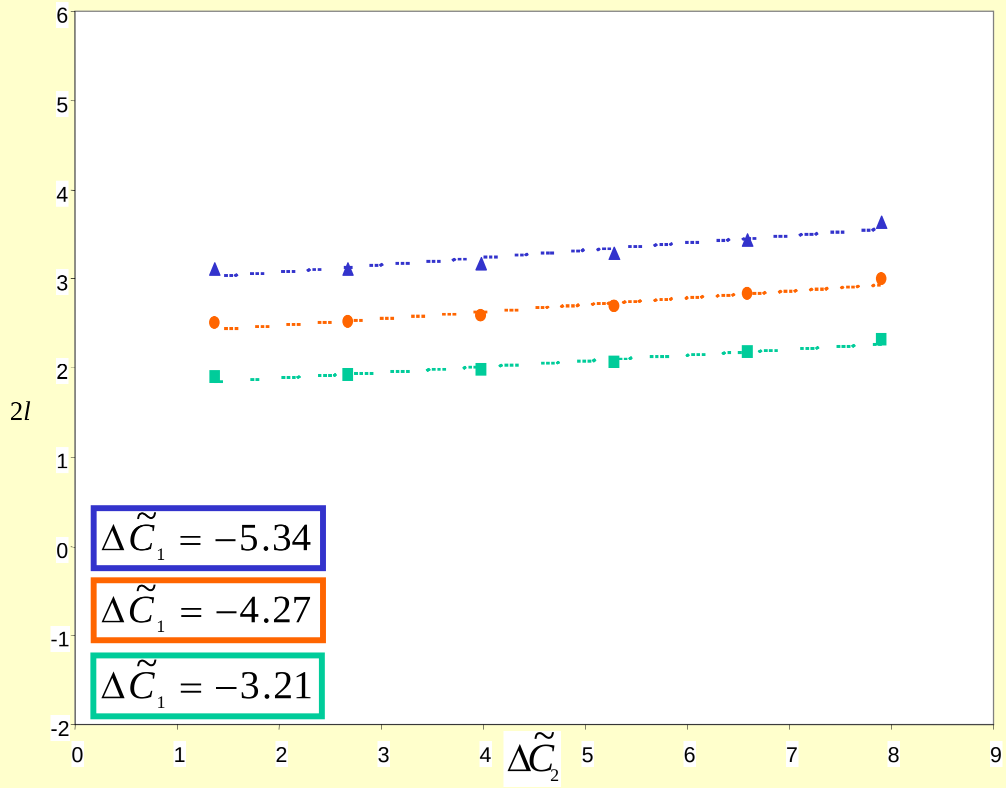
If $\Delta e_1^{Right} > 0$, then $l^{Right} \cdot \Delta\tilde{C}_1 < 0$

If $\Delta e_1^{Right} < 0$, then $l^{Right} \cdot \Delta\tilde{C}_1 > 0$

Variation of "Horns" with Composition

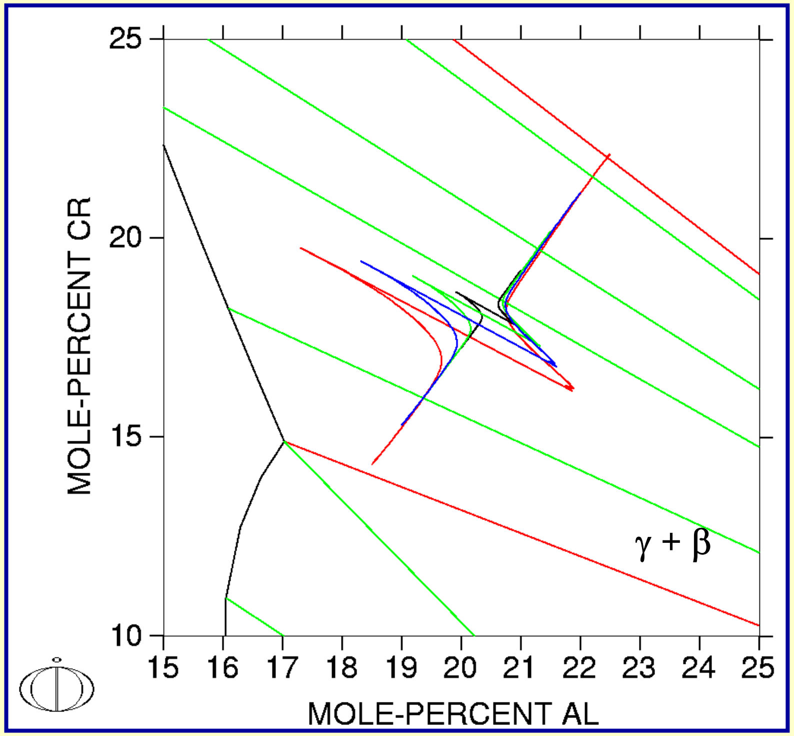
$\Delta\tilde{C}_1 = -4.27$

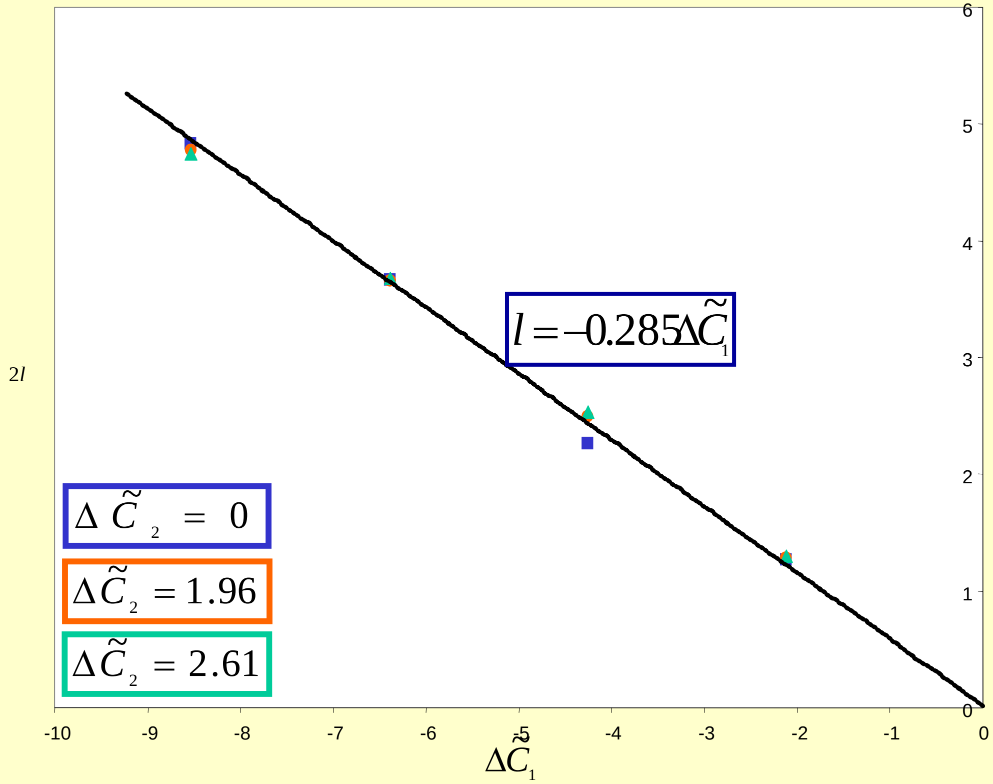




Variation of "Horns" with Composition

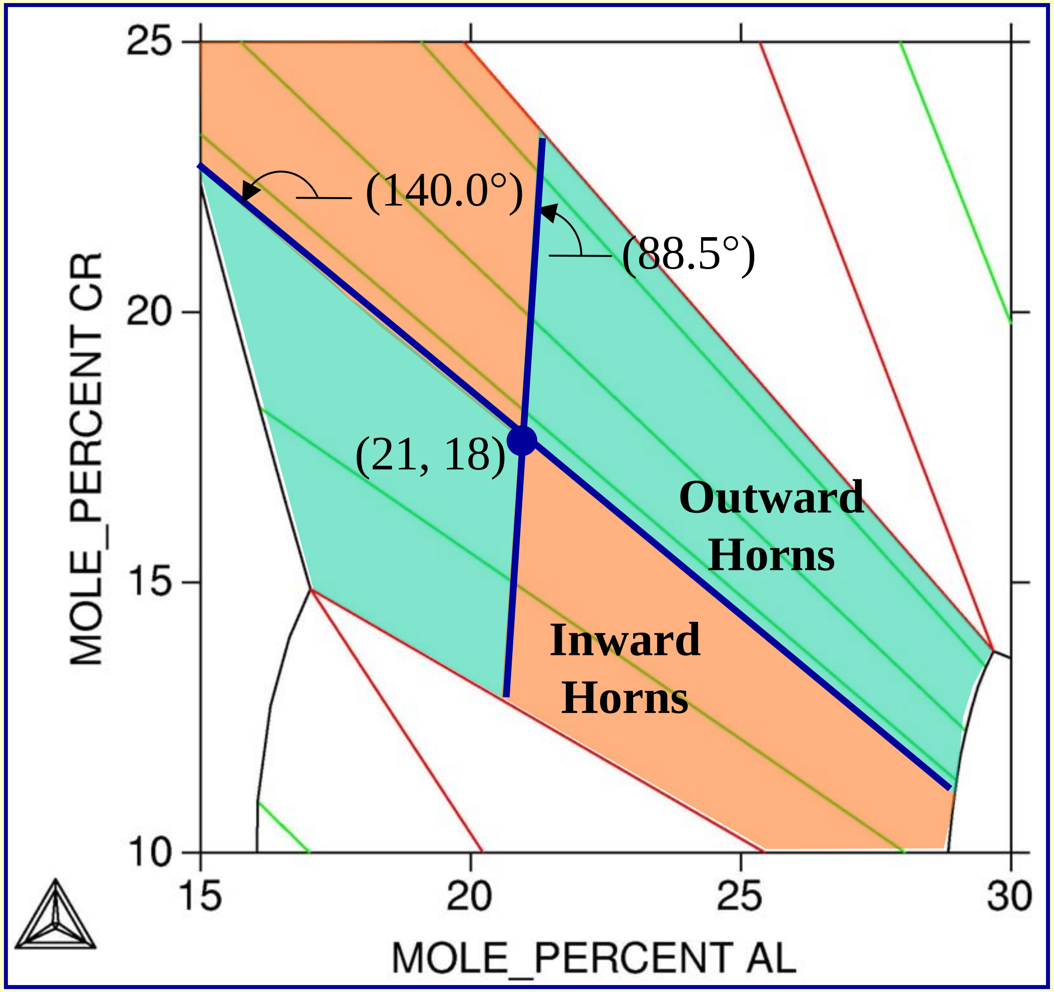
$\Delta \tilde{C}_2 = 0$



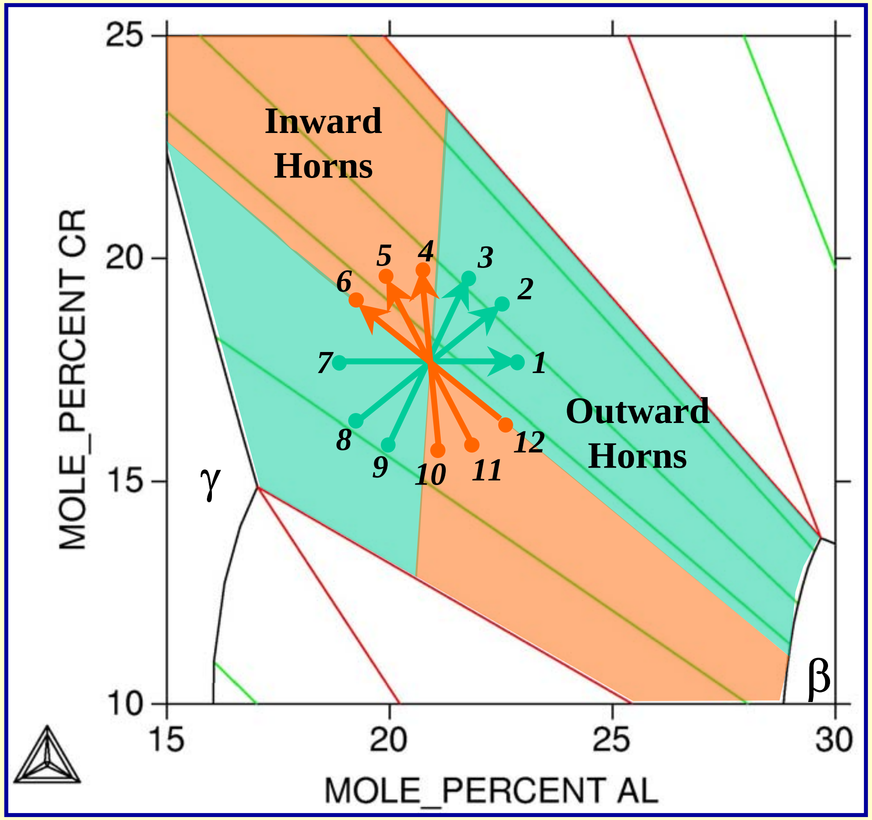


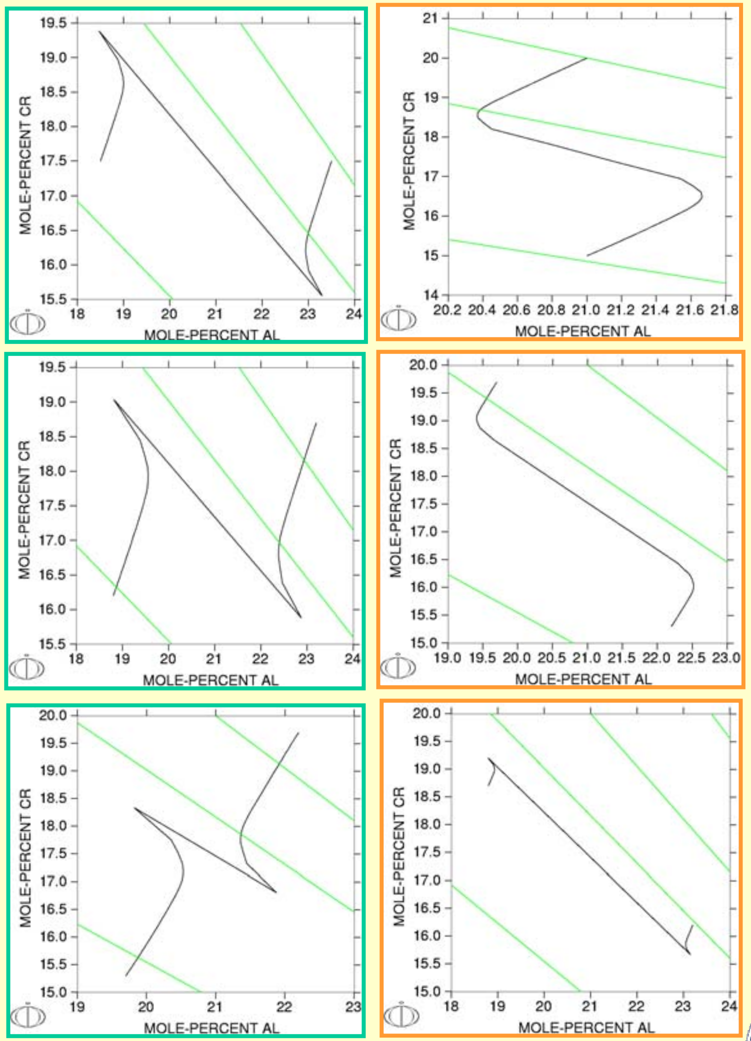
Variation of "Horns" with Composition

Transition between inward and outward "horns"



Variation of "Horns" with Composition





Summary

- **DICTRA simulations of two-phase ternary diffusion couples show sharp deviations from the linear zigzag paths, appearing as double or single horns.**
- **The double-horn has the same signs of the horn length for both left and right sides while the single-horn has the opposite signs.**
- **The type of horns may be predicted based on the relative position of two major eigenvectors and the position of the composition vector.**
- **The horn length varies linearly with the component of the composition vector along the major eigenvector direction of the diffusivity matrix.**

Acknowledgements

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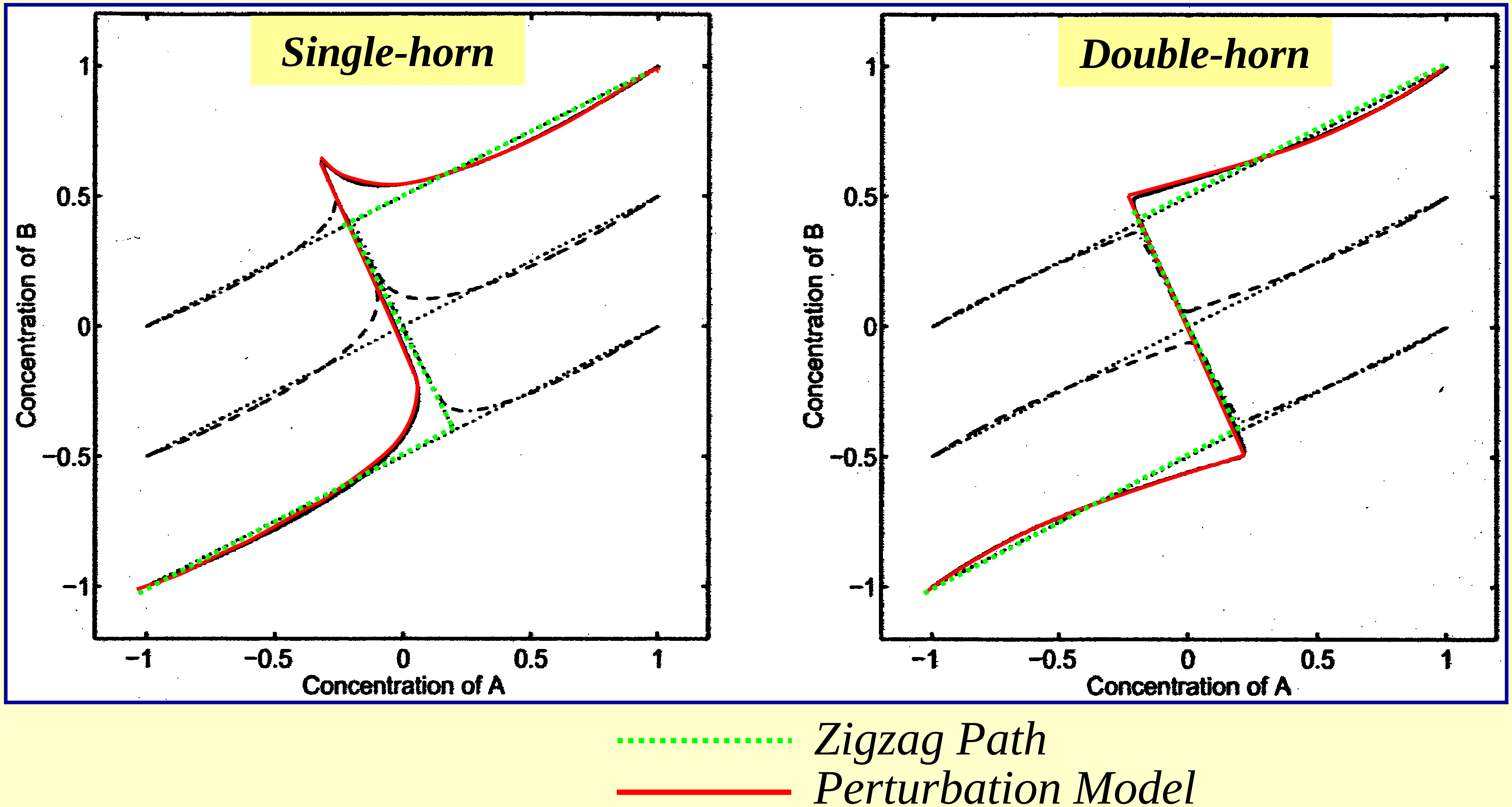
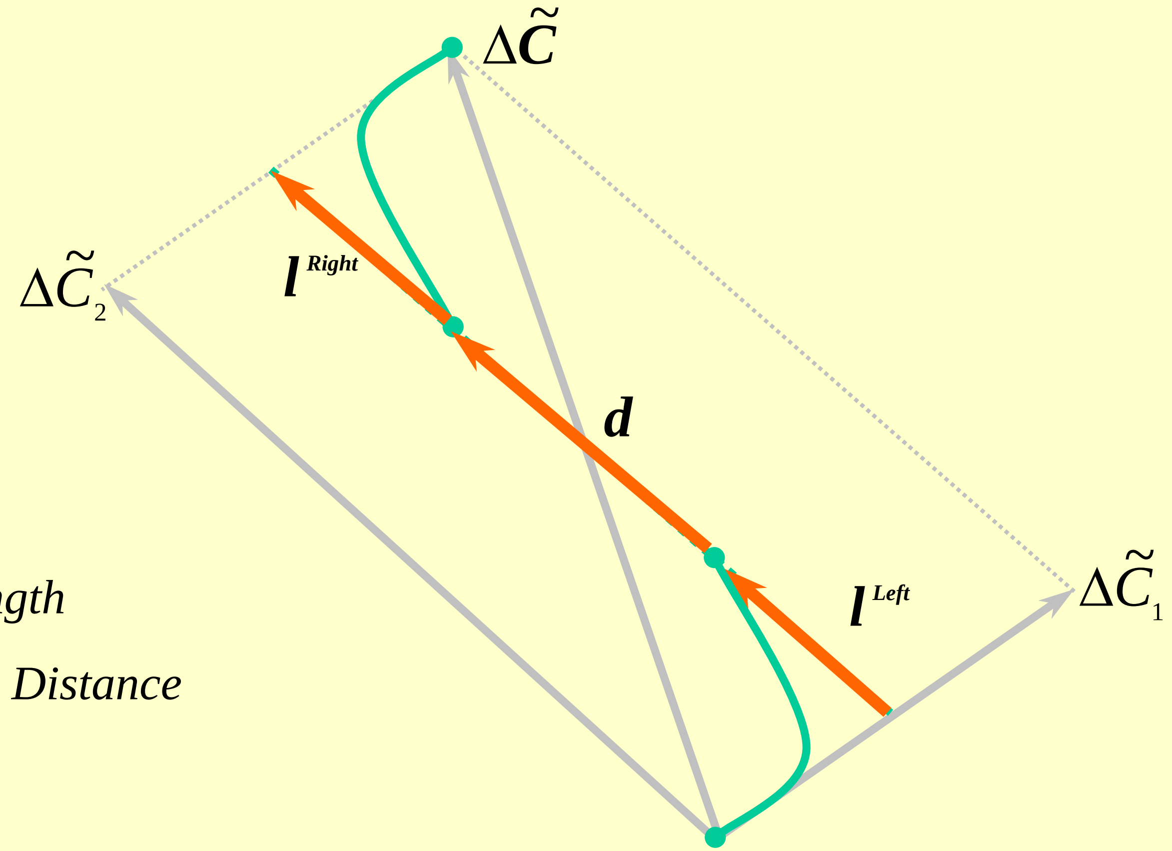
Diffusion Paths from Perturbation Model



* M. Schwind, T. Helander and J. Ågren, Scripta. Mater. 44(2001) 415-421

Variation of "Horns" with Composition

Relation between the horn length and the horn tip distance



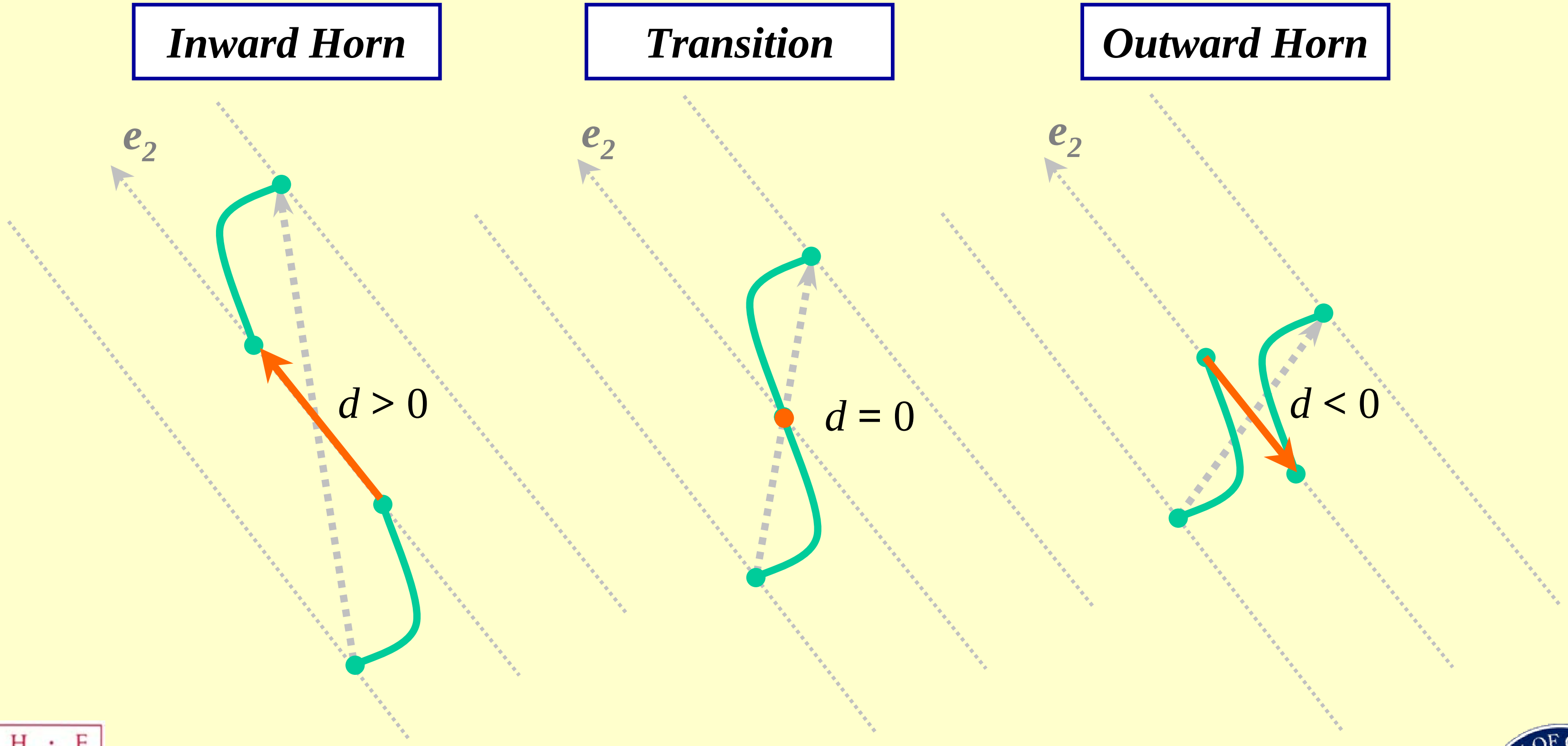
l: *Horn Length*

d: *Horn Tip Distance*

$$\boxed{d = \Delta\tilde{C}_2 - 2l}$$

Variation of "Horns" with Composition

Transition between inward and outward "horns"



Diffusion Paths from DICTRA Simulation

Two-phase Ternary Diffusion Path

- Linear
- Non-linear
  - Single-horn
  - Double-horn
    - Outward
    - Inward