Dendritic Core Crystallization in Minor Planets - an empirically constrained simulation study

Agpalilik mass

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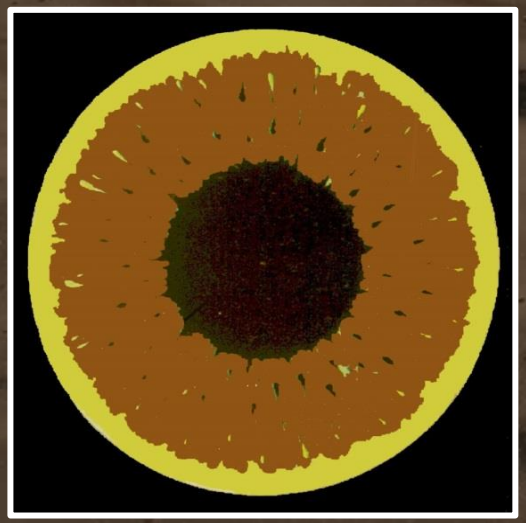

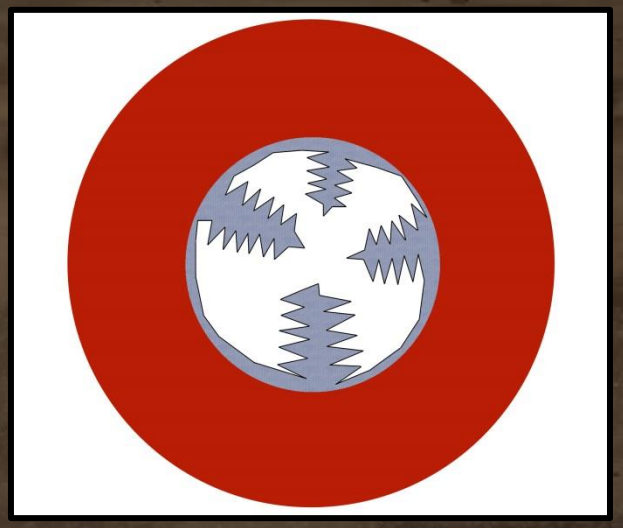

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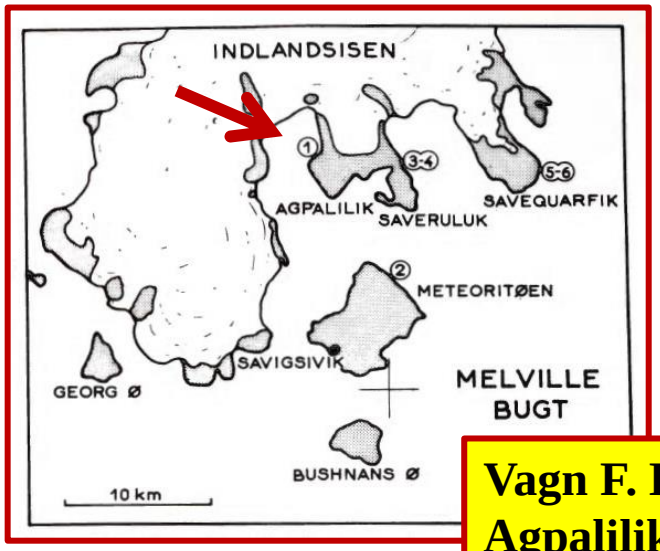

Vagn F. Buchwald – discovery of the Agpalilik mass (1963) - a meteorite saga

Composition - Ni: 7.58%; Ga 19.2 ppm; Ga, Ge 36.0 ppm

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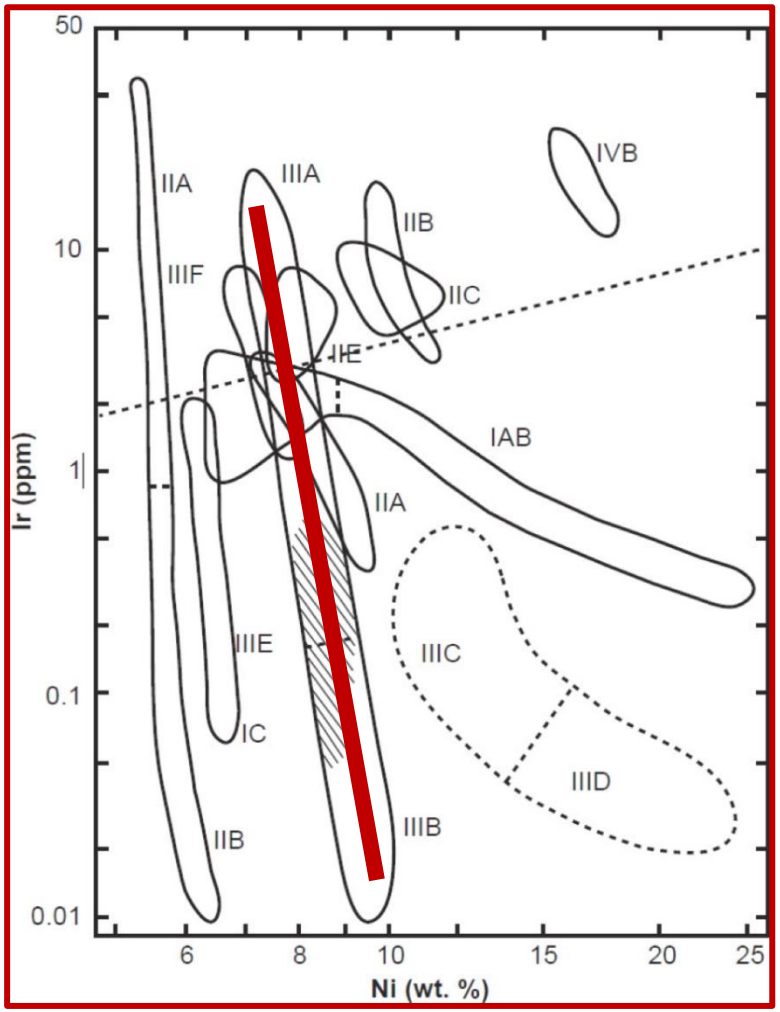

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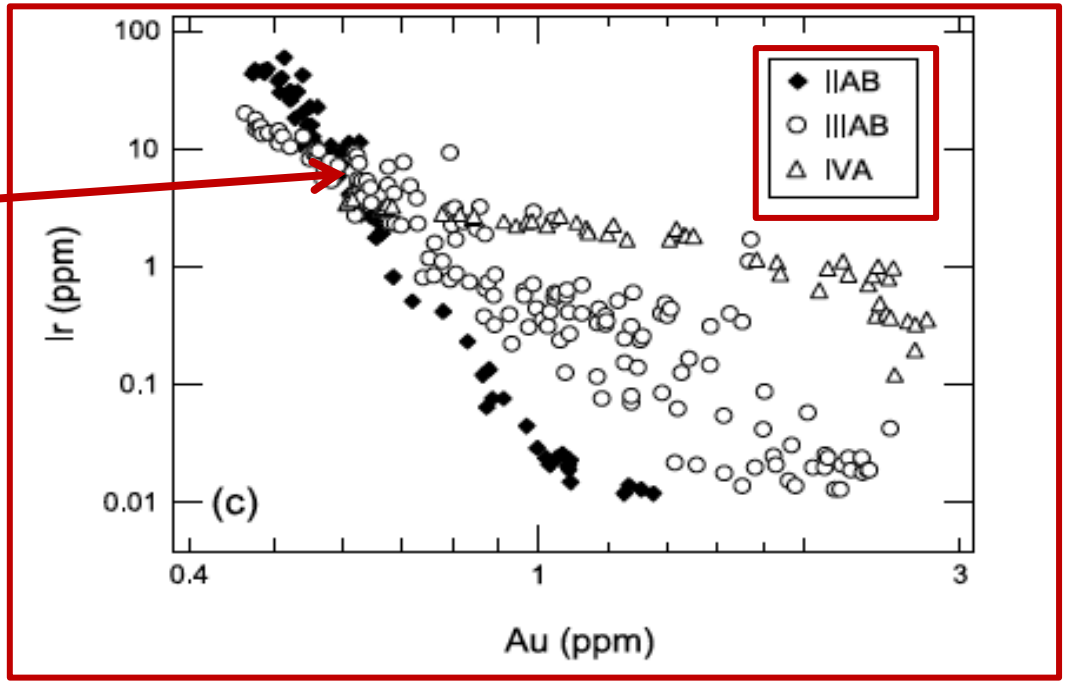
Agpalilik mass

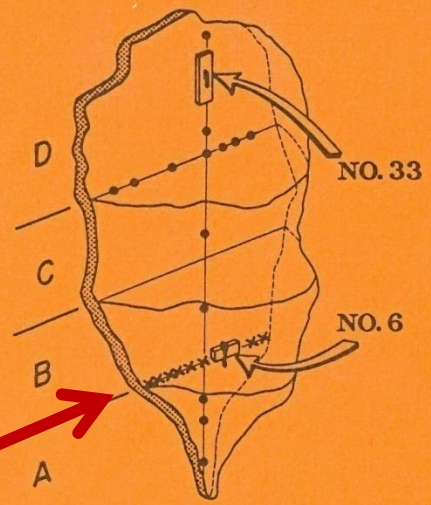


Au versus Ni concentrations in iron meteorites from three different asteroids. The first solid to crystallize was rich in Ir and low in Au. N.B. as crystallization progresses to the right, Ir concentrations become more and more diverse. The different slopes seen in the three groups are due to different sulfur concentrations in the cores. Sulfur controls the distribution of the elements between liquid and solid metal. (From Chabot and Haack, 2006)

KIM H. ESBENSEN

CHEMICAL AND PETROLOGICAL STUDIES IN IRON METEORITICS

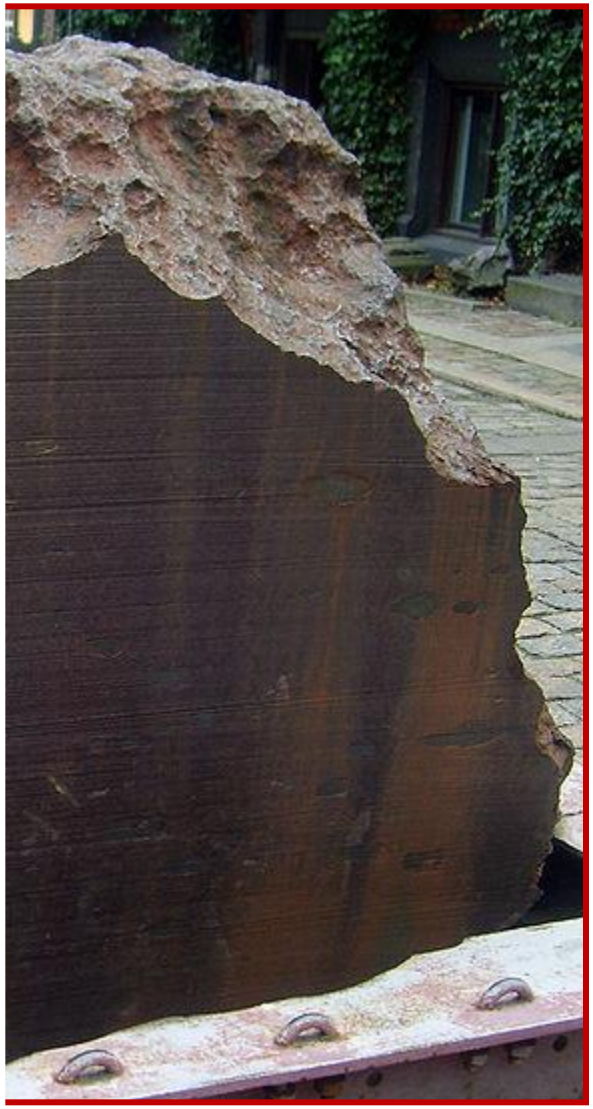
Ph.D. Thesis



Cape York, Agpalilik

DEPARTMENT OF METALLURGY

THE TECHNICAL UNIVERSITY OF DENMARK



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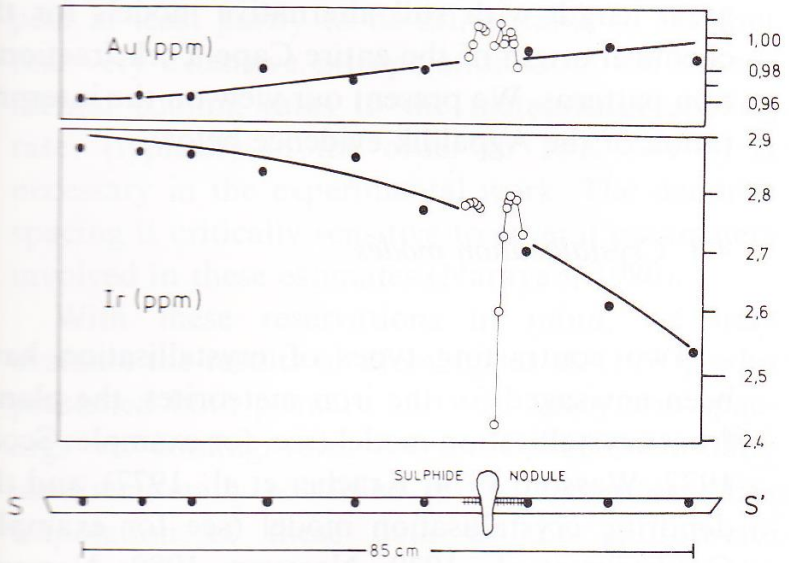
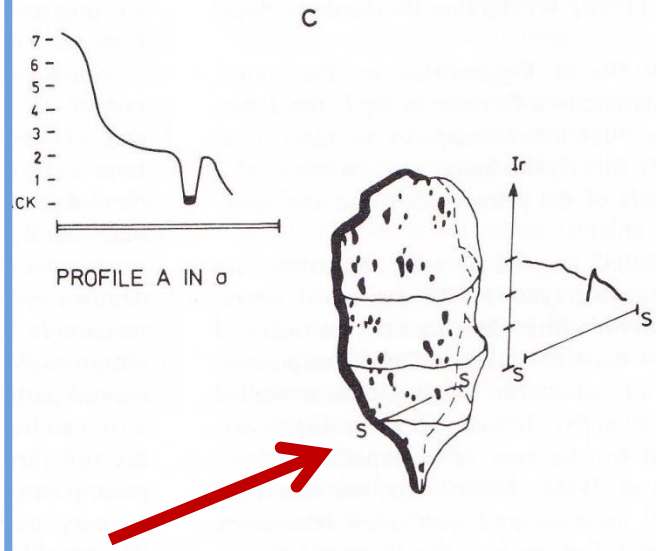


Fig. 3. Transverse chemical gradients in the Agpalilik metal. S–S′ section across the Agpalilik slab presented in Fig. 2 with detailed sample locations, dimensions etc. Two types of trends are present: (1) A 'macrofractionation' trend (filled circles–thick, solid trace) across the entire slab, and (2) a 'microfractionation' trend (open circles–light, solid trace) only close to one troilite nodule, where sampling is very closely spaced. Both Ir and Au show a significant, systematic macrofractionation trend of opposite character (depleted–enriched from left to right, respectively), interpreted in the text as representing transverse dendritic growth during passage of the contemporaneous crystallisation front, parallel to $[100]_\gamma$ (the *Y*-direction) through the volume element now occupied by the Agpalilik mass. The microfractionation trend is attributed to liquid entrapment between primary and tertiary dendrite arms (see Fig. 8). Cotectic metal–troilite precipitation most probably corresponds only to the two innermost (opposite) samples right up to the troilite nodule.

Interpretation: ”Transverse thickening” of a primary, or a tertiary dendrite arm .....



atural dendritic fractionation patterns: (a) A 196× magnified section parallel to m Singh et al. (1970, fig. 5). Note how the eutectic is preferentially concentrated ental system. Contours (wt% Al): (7) 98.00; (6) 97.75; (5) 97.50; (4) 97.25; (3) 97.00; in (a) for comparison with (c) Ir-profile parallel to primary and tertiary arms in the trends in (b) and (c), disregarding the primary dendrite segment, present as the g segment was not sampled by the present Agpalilik volume, due to the very large f magnitude greater than the sampled section. In the text we argue for a genetic lendritic fractionation.

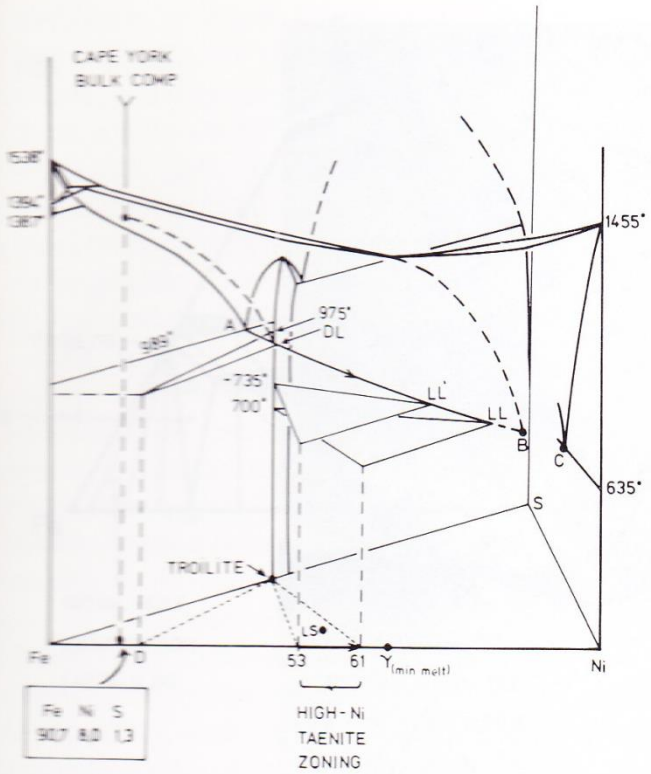
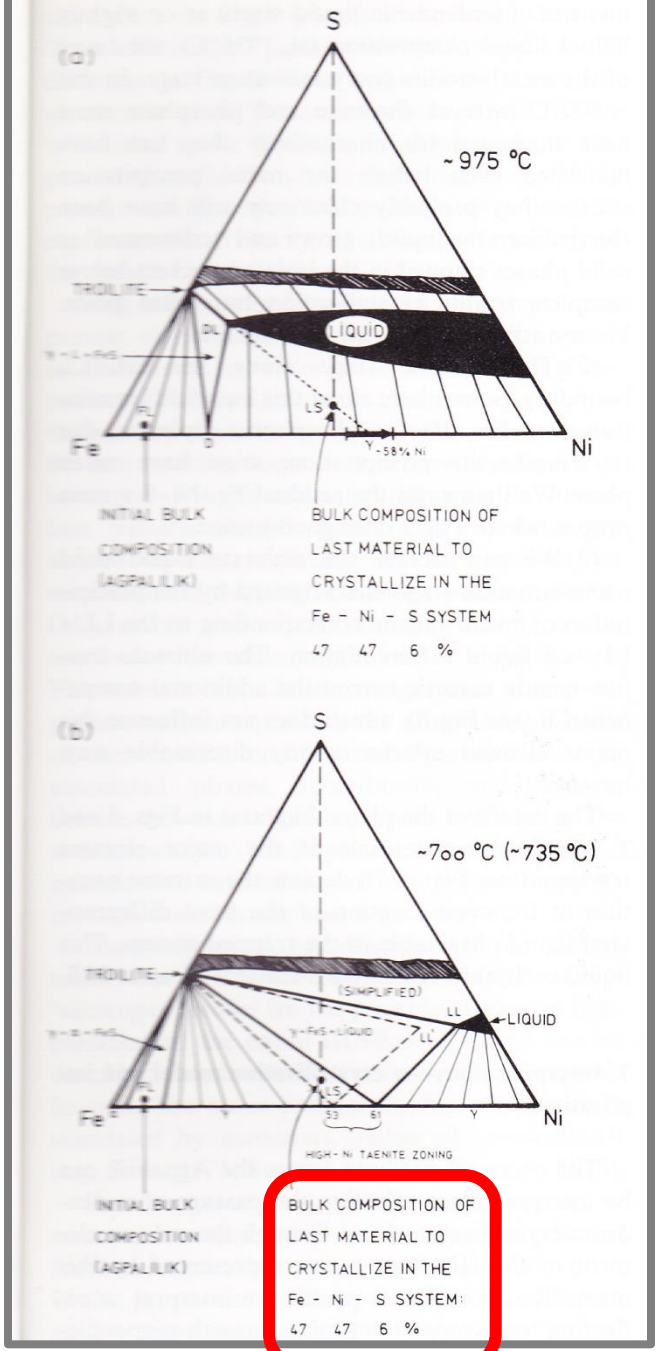


Fig. 5. Phase relationships in the Fe–Ni–S system above ~ 700°C. This system pertains to the entire fractional crystallisation of the Agpalilik meteorite, spanning a range of liquidus temperatures from ~1350 to 700°C. The corresponding liquid differentiation is routed from the initial bulk Cape York composition via DL through LL ('last liquid'). Composition LS represents the 'last solid' crystallisation product, the troilite–taenite eutectic further elucidated in Figs. 6 and 7. B represents the lowest possible temperature/composition of the cotectic metal/troilite boundary AB before appearance of ternary phases (not observed in the Agpalilik meteorite). The initial dendritic crystallisation of the Fe–Ni alloy takes place in the interval ~1350–975°C as the liquid differentiates to composition DL. Interdendritic entrapment (see Fig. 8) occurs just before and penecontemporaneously with this onset of cotectic metal–troilite precipitation judging from textural and chemical



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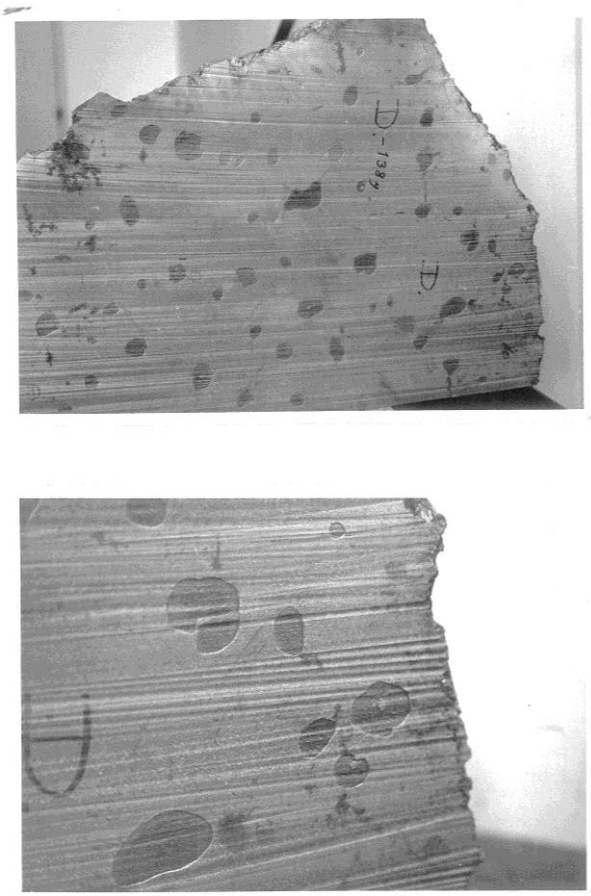

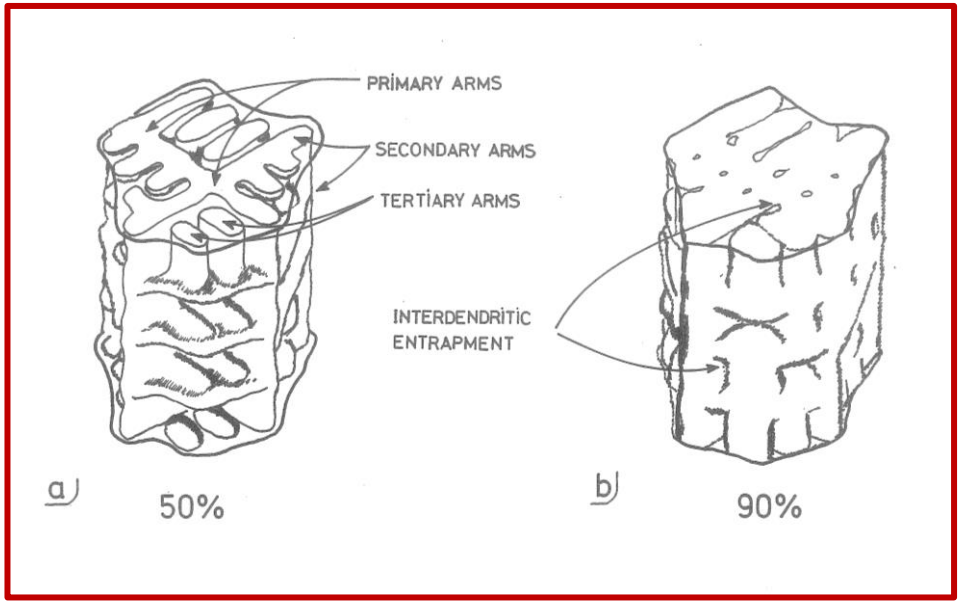

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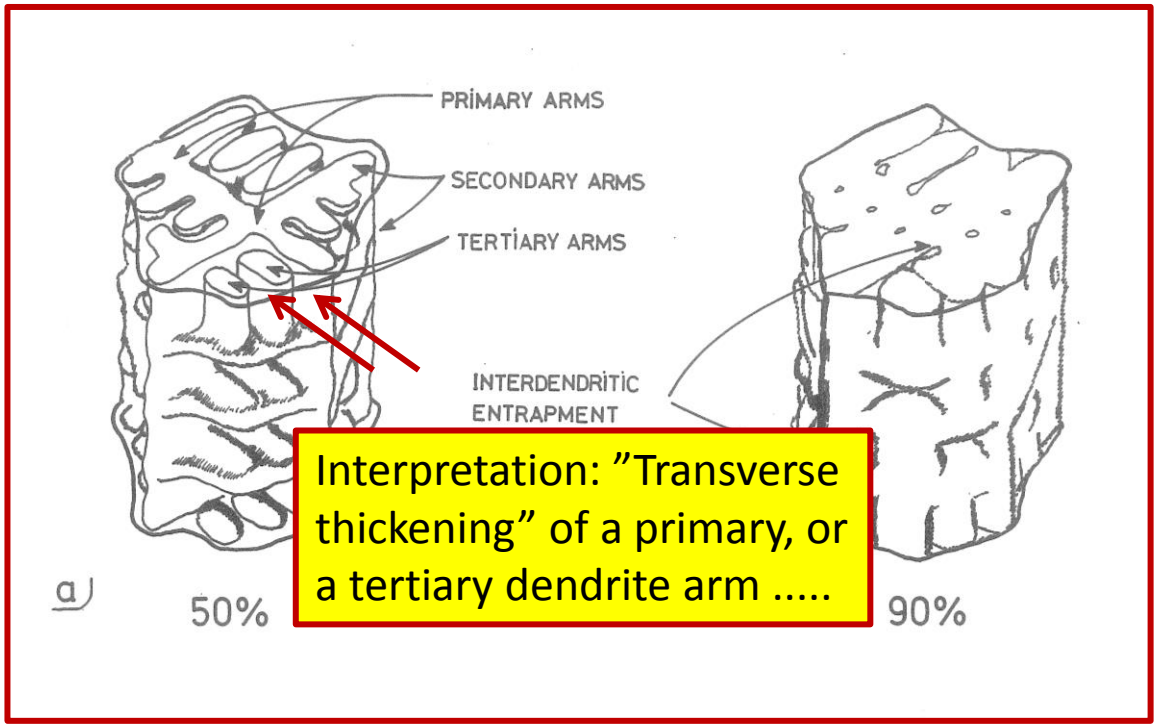
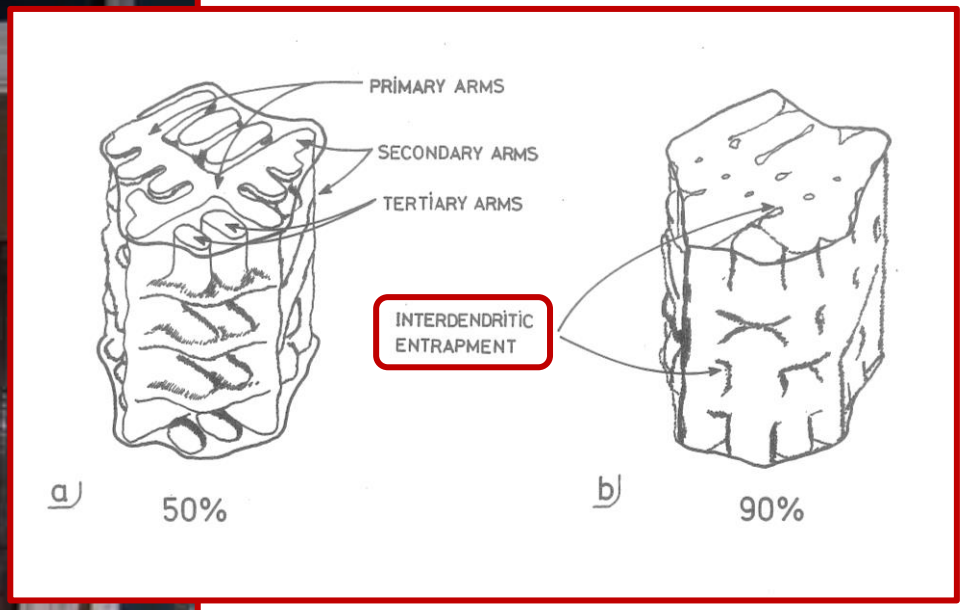


Interpretation: ”Transverse thickening” of a primary, or a tertiary dendrite arm .....

Planetary ”down”

Planetary ”up”



Interpretation: Direction of a primary, or a tertiary dendrite arm .....

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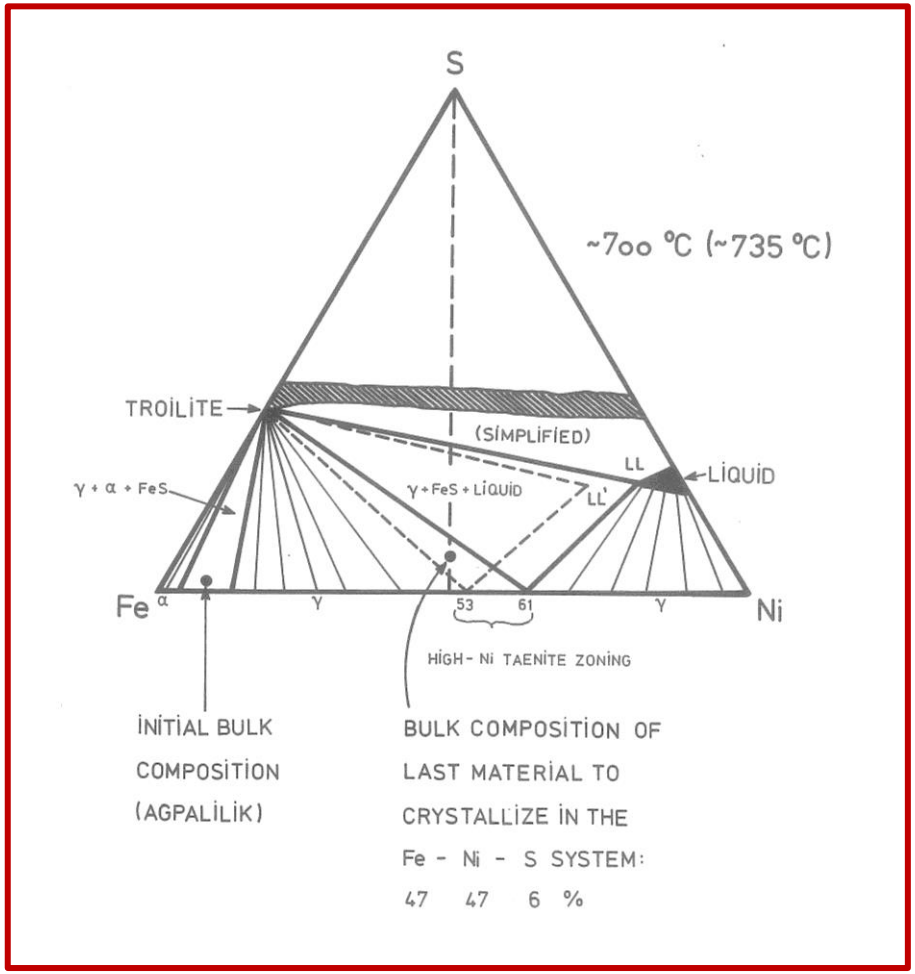
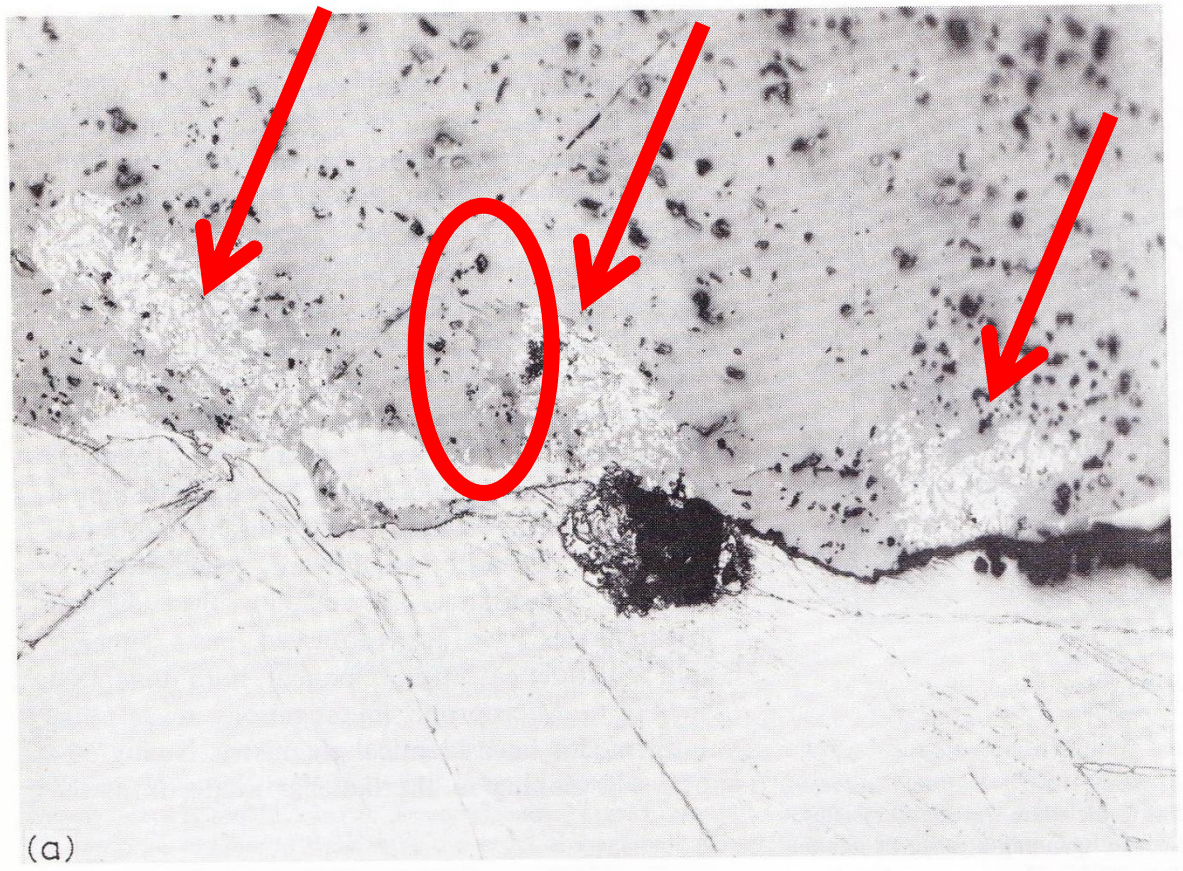
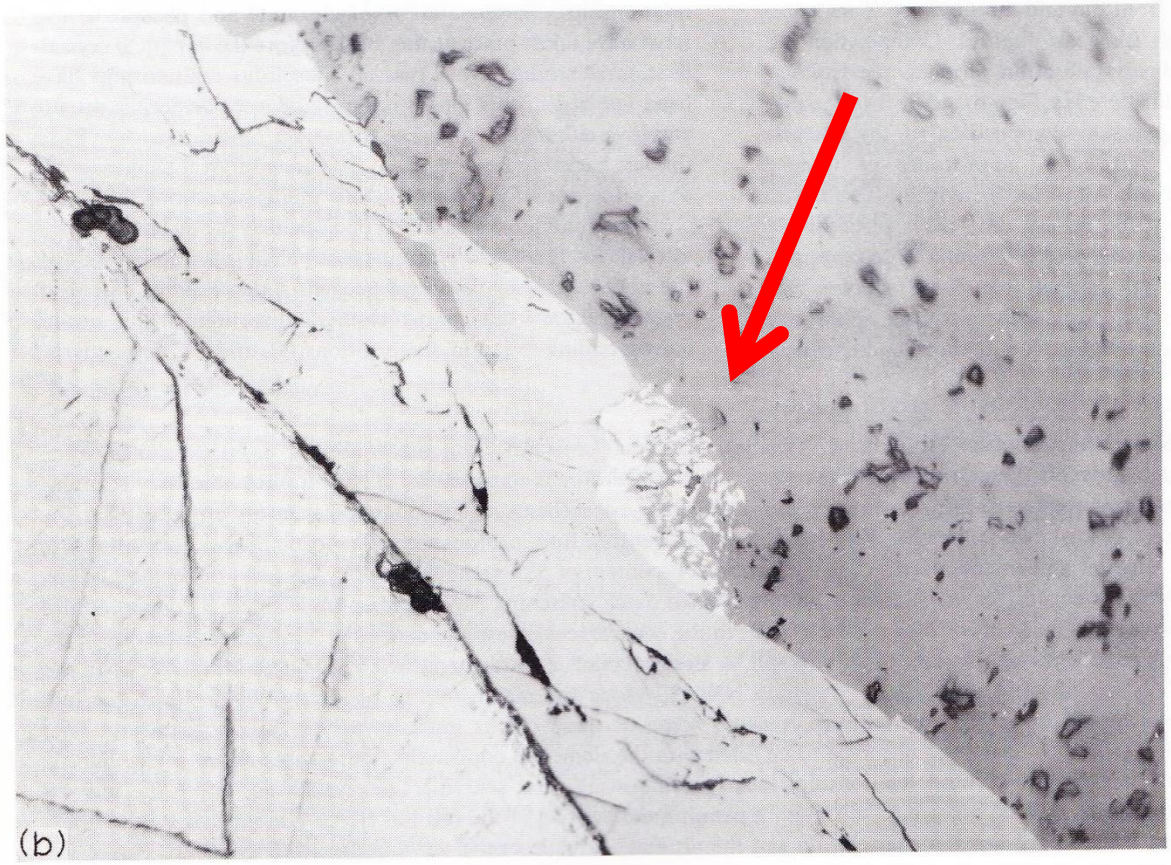



(a)


(b)

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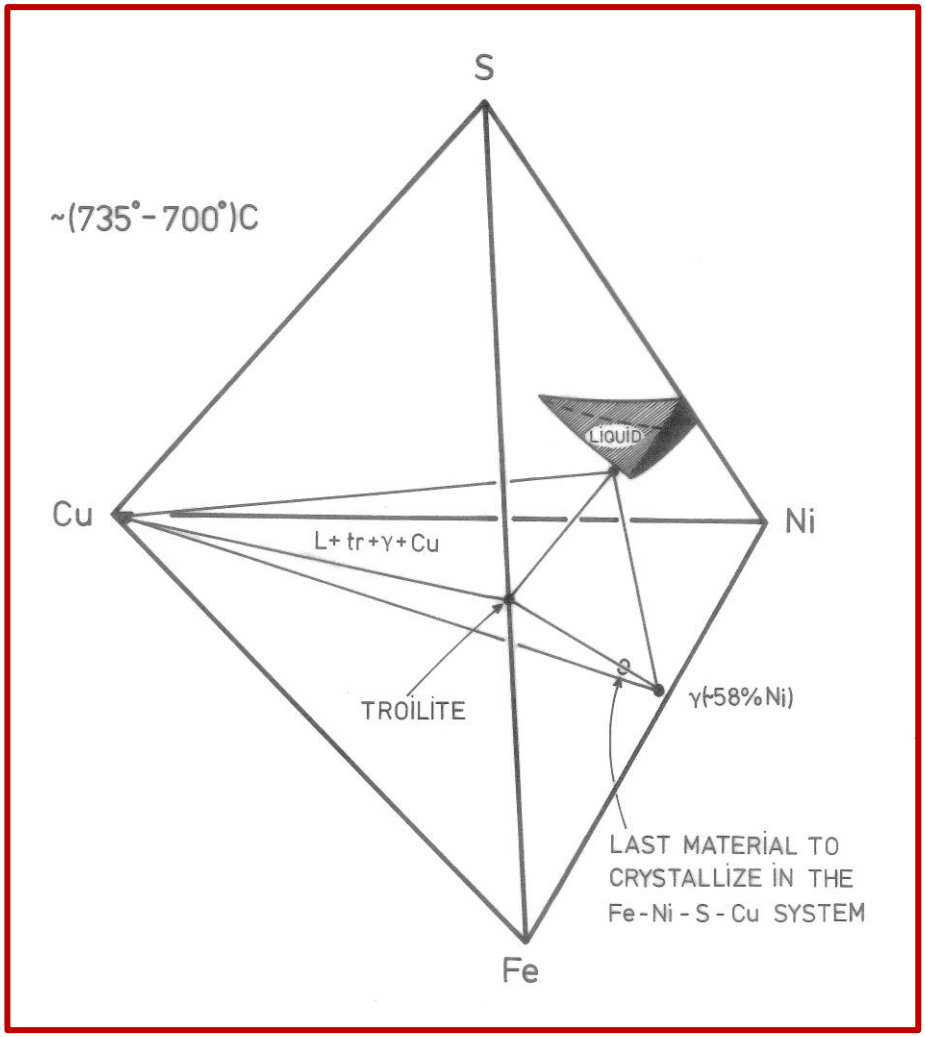

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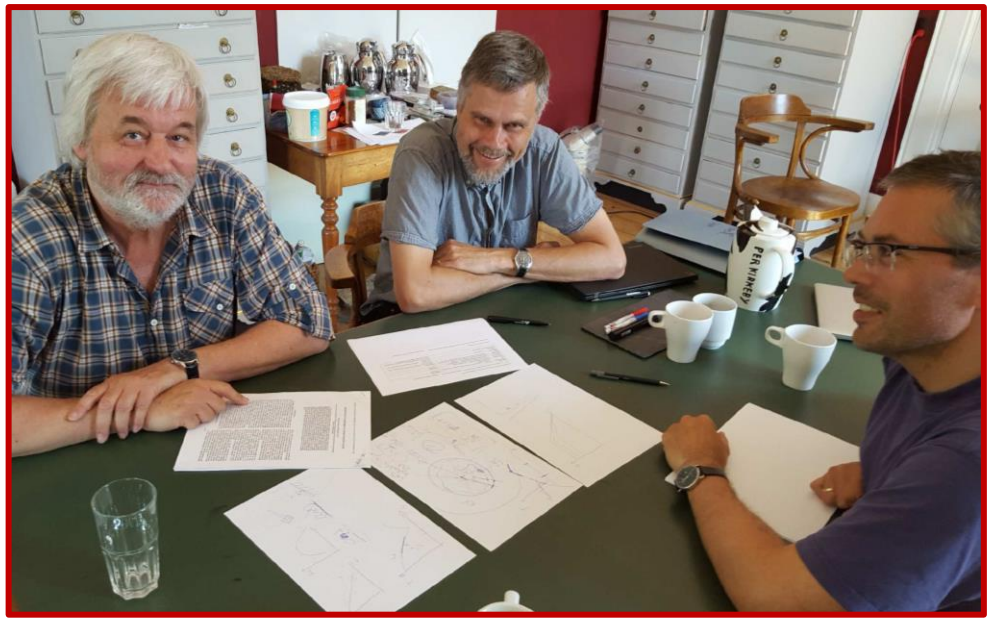

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Problem statement - Numerical modelling

Based on current iron meteorite understanding and using the newest iron meteorite compositional data to constrain the thermodynamics governing asteroid core crystallization, a.o. invoking effects of magnetic fields, pressure, cooling rate, rotation rate, core radius, a "blue-print" for a numerical simulation model of the crystallization of the Fe-Ni-P-S system will be established.

The simplest, comprehensive mathematical model of asteroid core thermodynamics must take into account both diffusive and convective heat transfer and the mechanics of a multi-component liquid mixture.

Hence the governing equations read:

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Mixture model of multiphase flow:

$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \boldsymbol{u}_k) = \Gamma_k$ (continuity equation), where α_k is the volume fraction of phase k, ρ_k is its density, $\boldsymbol{u}_k$ is its average velocity, and Γ_k is its rate of production. $\frac{\partial}{\partial t}(\alpha_k \rho_k \boldsymbol{u}_k) + \nabla \cdot (\alpha_k \rho_k \boldsymbol{u}_k \boldsymbol{u}_k) = -\alpha_k \nabla p_k + \nabla \cdot (\alpha_k \boldsymbol{\tau}_k) + \alpha_k \rho_k \boldsymbol{g} + \boldsymbol{b}_k$ (momentum equation), where p_k is the pressure of phase k, τ_k is the sum of its viscous and turbulent stress tensors, $\boldsymbol{g}$ is gravitational acceleration (which is non-constant, and has to be calculated from Newton's law or Gauss' law) and $\boldsymbol{b}_k$ is the sum of remaining body forces acting on phase k, such as Coriolis force (if rotation is taken into account).

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Heat diffusion and convection:

$\frac{\partial T}{\partial t} + \nabla \cdot (\boldsymbol{u}T) = \nabla \cdot (\kappa_i \nabla T)$, with boundary conditions at the solidification front $T = T_{melting}$ and $Lv_n = -\left[\kappa_l \frac{\partial T_l}{\partial \boldsymbol{n}} - \kappa_s \frac{\partial T_s}{\partial \boldsymbol{n}}\right]$ (moving boundary condition). Here subscript *l* denotes the liquid phase and *s* – the solid phase, *T* is temperature, κ is the thermal diffusivity, $\boldsymbol{n}$ is the normal vector to the solidification front, and v_n is the normal component of the velocity of the solidification front. This is also known as the classical Stefan problem.

Note that all of material constants are functions of the *local composition*, and have to be obtained from experimental data (e.g. phase diagrams for Fe-S mixtures). Special care has to be taken when coupling those two equations and designing appropriate boundary conditions at the liquid-solid interface, since crystallization process locally changes the volume fractions of individual components.

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Simulation approach

The relevant length scales in core crystallization span from centimeters (length scale of the smallest dendrites) up to tens and perhaps hundreds of kilometers (the radius of an asteroid). Simulating a complete asteroid core model at full resolution would be prohibitively imprac tical, hence we intend to apply the following simplifications in the first implementation:

1. Simulate a 2-D cross-section of an asteroid. While this will neglect transverse flow features inside the core, we believe that a 2D simulation can provide qualitatively good results, and will be able to shed light on troilite formation at a significantly lower computational cost. An extension to 3D is possible in principle, but is distinctly out of the scope of the present project.

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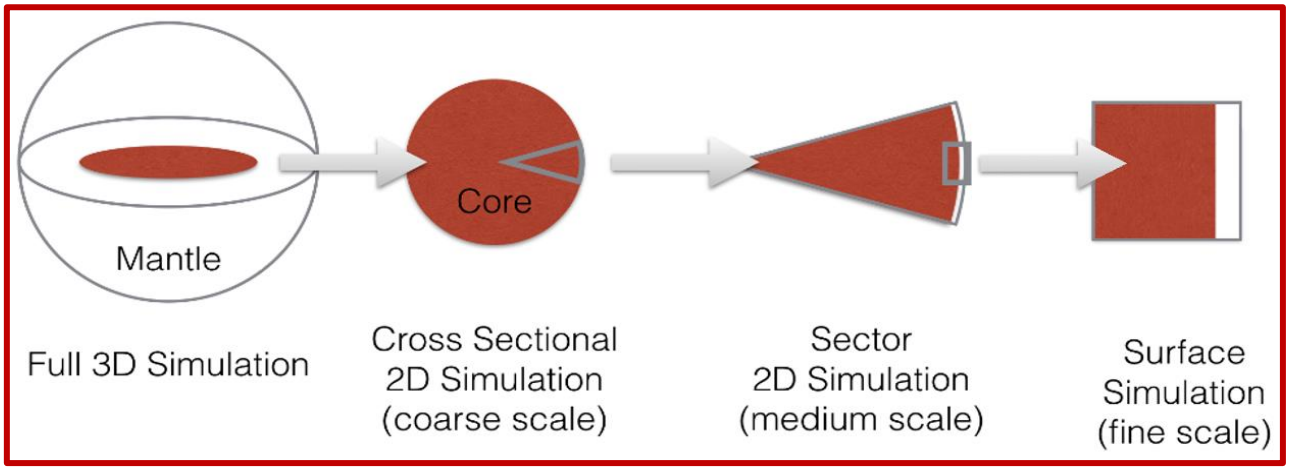

2. Use of a multi-scale model. Rather than maintaining a high-resolution representation of an entire asteroid, simulations will be performed at three different scales: coarse scale (entire asteroid) used to analyze the large-scale thermodynamics of the liquid core; medium scale (a single narrow radial sector of the core), and fine scale (a small area around the solidifying surface commensurate with the volume of the Agpalilik mass), used to model the ultimate details around the solidification front. This, we believe, will allow us to portray the global evolution and distribution of key chemical elements inside crystallizing core … ending with the ultimate inter-dendrite dendritic features.

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Simulate Fe-S core

3. While being able to keep track of full chemical composition of the core melt is certainly of interest, initially we will focus our attention to two-component iron-sulfur mixture. This will reduce the time needed to implement a proof-of-concept model prototype(s), as well as the computational cost of the model. Further, as we expect sulfur content to be the driving factor behind dendritic crystallization, this simplified model will allow us to draw first conclusions of this hypothesis in early stages of the project.

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Simplified fluid mechanics:

4. We begin with an assumption that the melt is an alloy and that the relative velocities of the two components (Fe and S) are negligible. This will only require us to solve a single-component Navier-Stokes equation, while the fluctuations in sulfur concentration can be modelled with an advection-diffusion equation. Further, we will use the Boussinesq approximation to the Navier-Stokes equation, i.e. an assumption that the fluctuations in density are small and only affect the flow through buoyancy forces. Such a model is sufficient to capture convective rolls formation inside a liquid, and an assumption of low variation in density is acceptable for small asteroids. Further simplifications might have to be made, considering that the large-scale flow inside an asteroid core is characterized by a Reynolds number on the order of 10^9, suggesting use of dedicated turbulence models.

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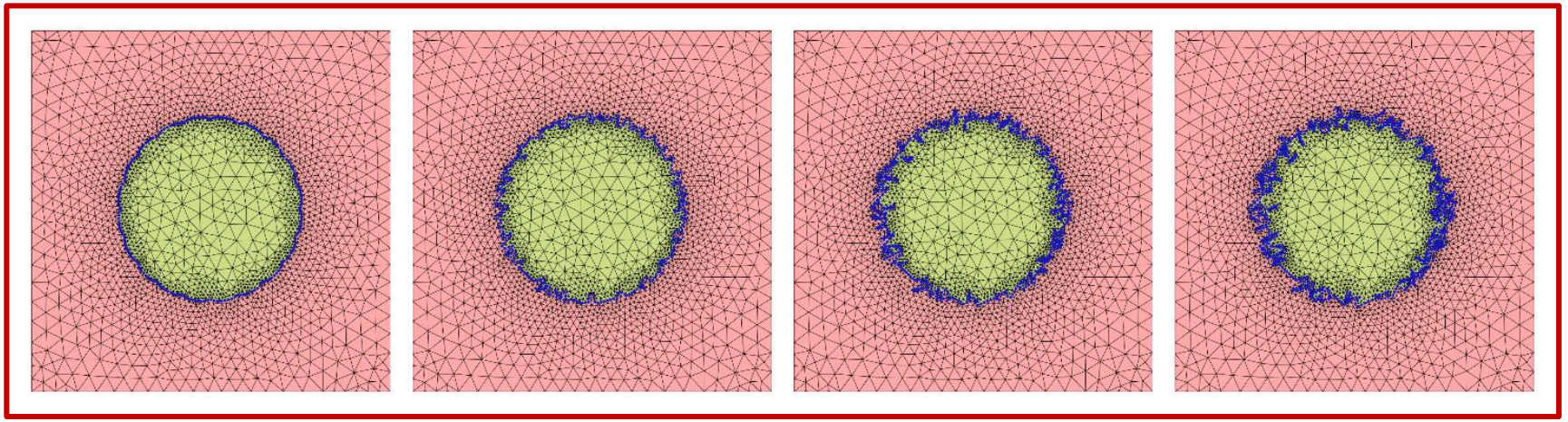

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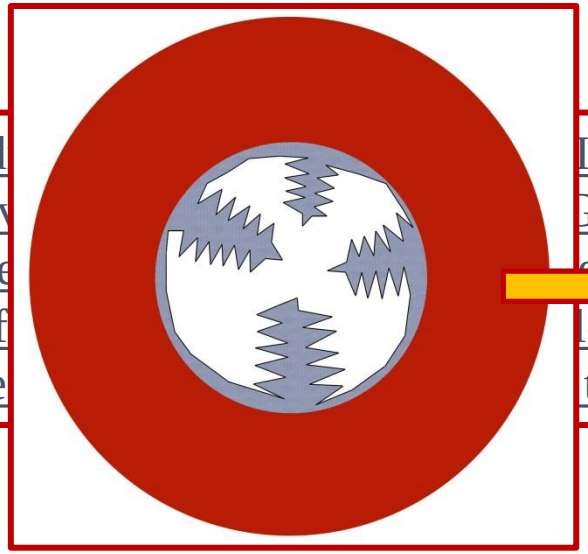

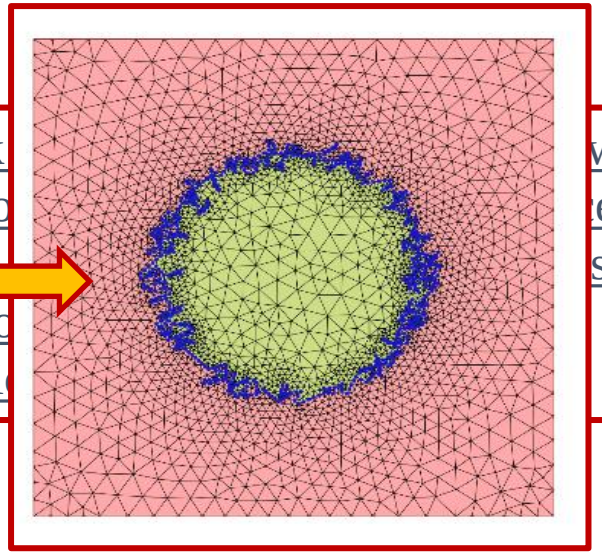

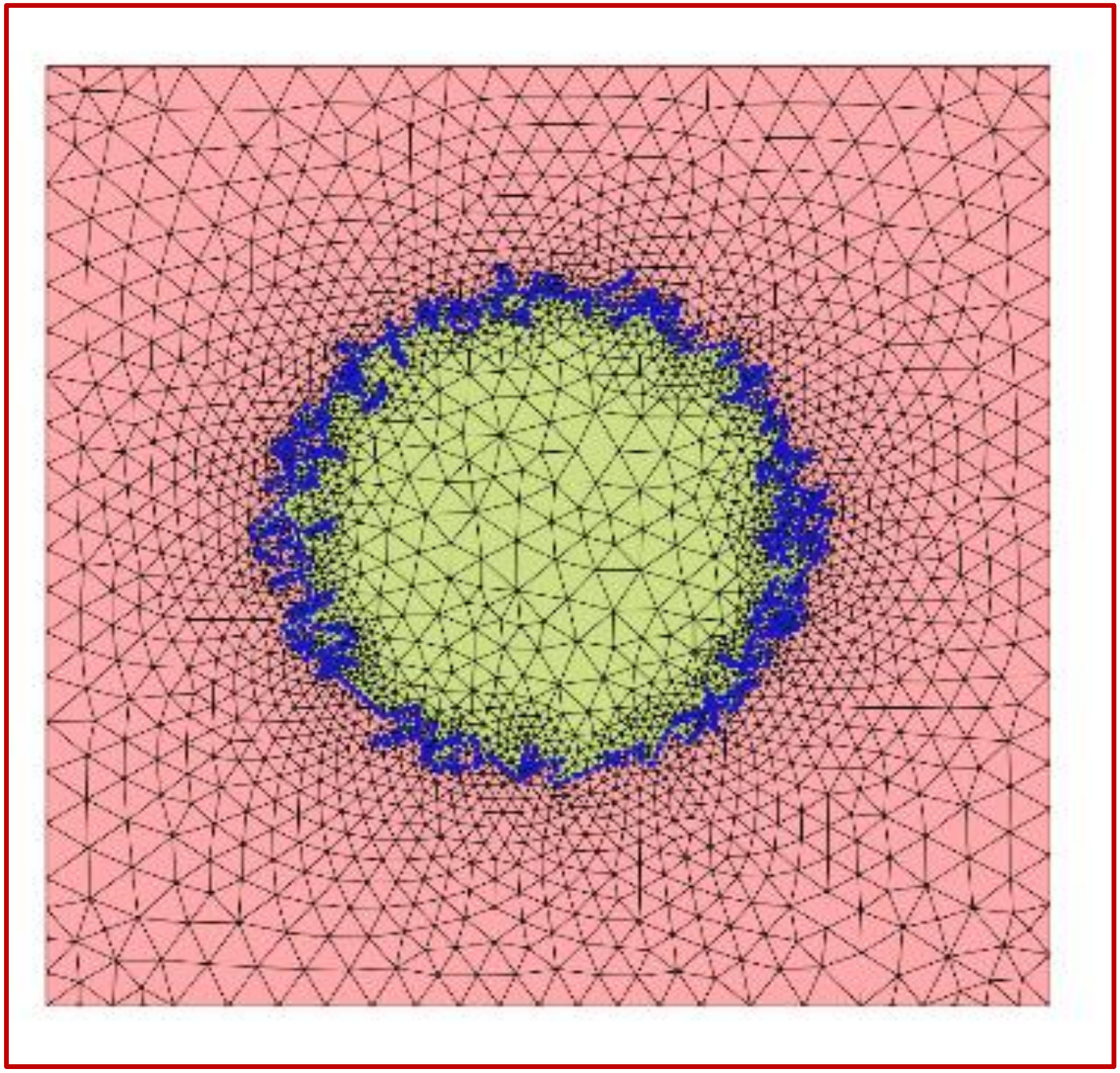

The hard core simulation crew

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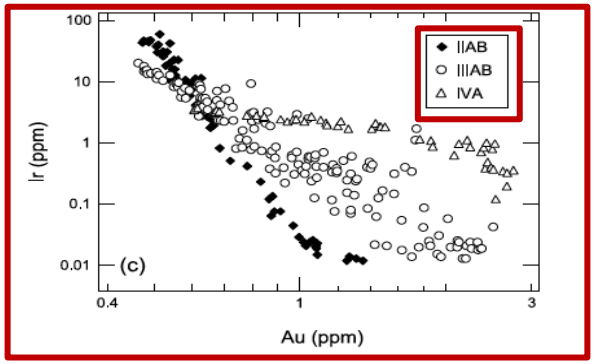
Effects of simplifying assumptions:

After successful completion of the **first** model implementation, we will study closer the effects of the simplifications included, with special focus on the core's chemical composition and its fluid mechanics.

Effects of simplifying assumptions:

After successful completion of the **second** model implementation, we will study closer the effects of the simplifications included, with special focus on the core's ***chemical composition*** and its fluid mechanics.



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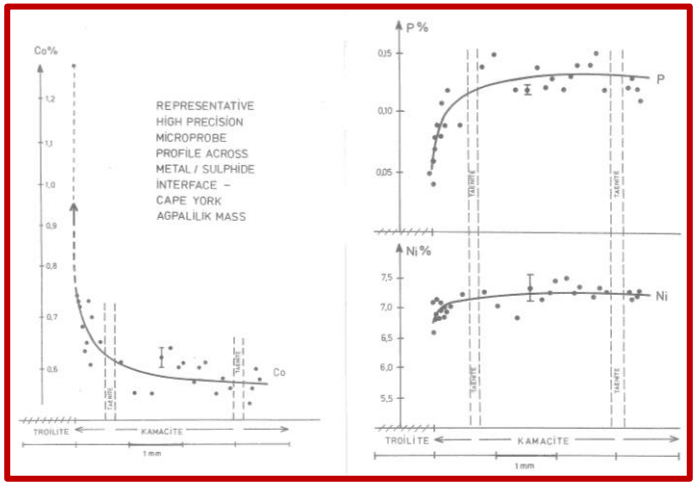
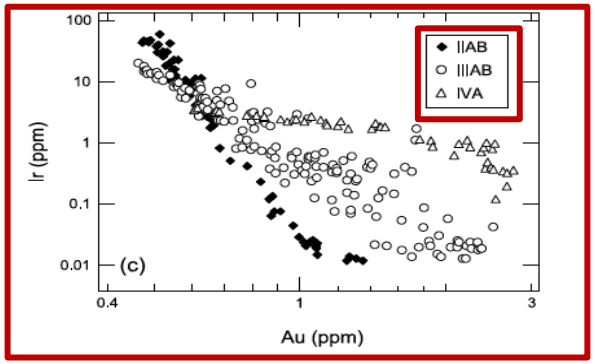
lots of interesting possibilities and implications …. for deeper understanding of early solar system smaller planetoid body differentiation …. → asteroids





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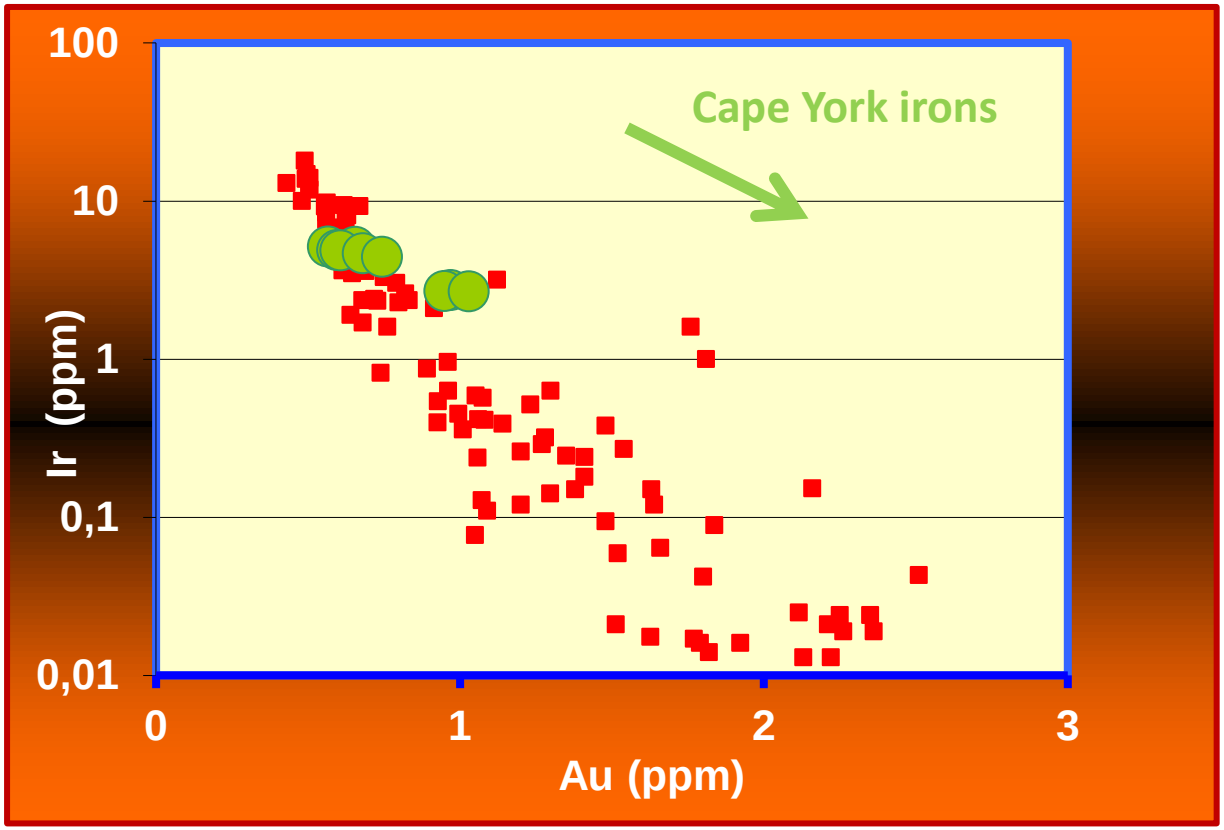

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Thank you for your attention ...

Hope very much to see you again at future Nordic Geological Winter Meetings (2019, 2021) ...

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