Upscaling from Mesoscopic to Macroscopic Solidification Models by Volume Averaging

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1. ABSTRACT

The mesoscopic solidification model is based on a simplified representation of dendritic structures by their envelopes. It provides quantitative predictions of dendritic growth over a wide range of solidification conditions. Because of its low computational cost compared to microscopic (e.g., phase-field) methods, parametric studies can be performed on a scale that corresponds to the Representative Elementary Volume (REV) used in deriving volume-averaged macroscopic models of solidification processes. In the present study, the mesoscopic model is applied to dendritic solidification of up to 100 interacting equiaxed grains. The results are averaged over the volume containing the grains and then used to obtain constitutive relations for macroscopic models. We present relations for the specific surface area of the grain envelopes and the solute diffusion length from the grains into the extra-dendritic liquid. It is shown that the present computational upscaling approach can be used to obtain improved constitutive relations.

Key Words: Alloy solidification, Dendritic growth, Multiscale modeling, Scale bridging

2. INTRODUCTION

The growth of dendritic grains is governed by an intricate interplay between diffusion and convection of heat and solute as well as capillary and surface effects. The growth is also influenced by adjacent grains. These can "feel" each other due to the overlap of thermal and solutal fields surrounding each grain. Dendritic structures can be simulated by (*microscopic*) phase-field methods. However, computing and memory requirements for these methods are heavy. It is only possible to apply them on the scale of a few dendrites and for purely diffusive situations on standard computers. Cellular-automaton modeling [1] is a common *mesoscopic* approach that can simulate the growth of multiple dendrites on a larger scale at the expense of simplifications. However, it is not able to predict accurate grain shapes and relies on very approximate relations for modeling grain interactions.

The mesoscopic envelope model [2] offers a complementary tool for the study of dendritic solidification. This model consists of the description of a dendritic grain by its envelope. The driving force for the envelope growth is linked to the solute concentration at a certain distance ahead of the envelope, the stagnant-film thickness. The branched dendritic structure inside the envelope is only implied and its details are not resolved; the interior of the envelope is rather described in a volume-averaged sense by fields of solid fraction and averaged phase concentrations (Fig. 1). This model has been validated and shown to provide physically realistic results for both equiaxed [3,4] and columnar [5,6] dendritic growth. It provides an accurate description of the envelope shape and growth velocity. The detailed level of the representation of grain interactions combined with the low computational cost makes the mesoscopic envelope model a promising tool for scale bridging approaches that would provide constitutive relations for macroscopic models. In this paper we show a first application of such an approach.
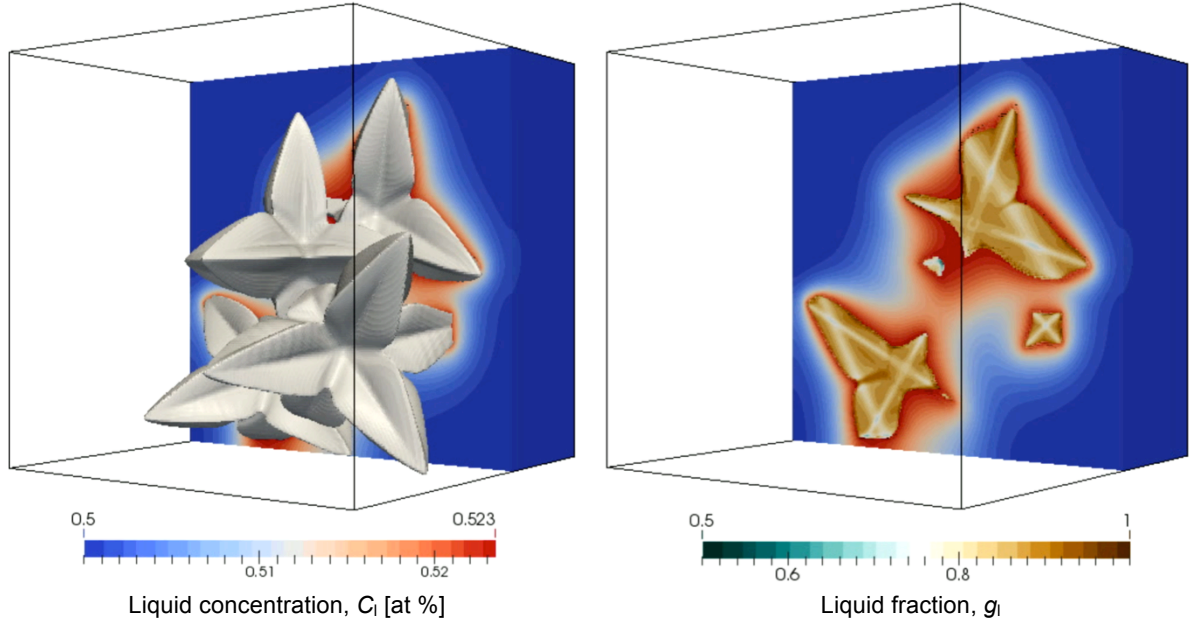
Fig. 1: Example of results of a simulation with the mesoscopic model. Left: four interacting equiaxed grain envelopes growing in an enclosure. Right: a slice across the enclosure showing the liquid fraction field in the interior of the envelopes and the concentration field in the liquid outside the envelopes. The initial supersaturation of the melt is Ω_0 = 0.05 and the composition is SCN-0.5 %acetone.

3. RESULTS

We used the mesoscopic envelope model to simulate a Representative Elementary Volume (REV) used in deriving volume-averaged macroscopic models of solidification. The results are averaged over the volume containing the grains and then used to obtain constitutive relations for macroscopic models. Fig. 2 shows simulations of randomly distributed and oriented grains growing isothermally in a cubic enclosure (the REV) at an initial supersaturation of Ω_0 = 0.05. Three different grain densities are considered. The dimensionless grain density, $N_V^{l\text{diff}}$ represents the mean number of grains in a volume of l_{diff}^3, where the characteristic length $l_{\text{diff}} = D_l/V_{\text{LGK}}$ is the diffusion length at the primary tip growing at the theoretical speed, V_{LGK}, at the initial supersaturation Ω_0. The theoretical tip speed is obtained from the Ivantsov solution combined with a tip selection criterion of the type $R_{\text{tip}}^2 V_{\text{tip}}$=const. In the presented simulations the mean distance between the grain centers, d_0, varies from 22 l_{diff} to 7 l_{diff}, resulting in different levels of solutal interaction. It is estimated based on a close regular packing arrangement (FCC or HCP) of the grains: $d_0=(N_V^{l\text{diff}}/\sqrt{2})^{-1/3} l_{\text{diff}}$. Note that in an isothermal configuration Ω_0 and $N_V^{l\text{diff}}$ are the only physical parameters and fully characterize the conditions of the system. As we can see in Fig. 2, the grains first grow freely. Later on, the overlap of diffusion fields slows down the primary tips and the envelopes continue to grow laterally, adapting to the adjacent grains. At a smaller mean distance between grains the interactions start earlier. The liquid between the envelopes (extradendritic liquid) is continuously enriched by the solute rejected from the envelopes. Finally, the concentration of the extradendritic liquid reaches the equilibrium liquid concentration and the growth of the envelopes stops.
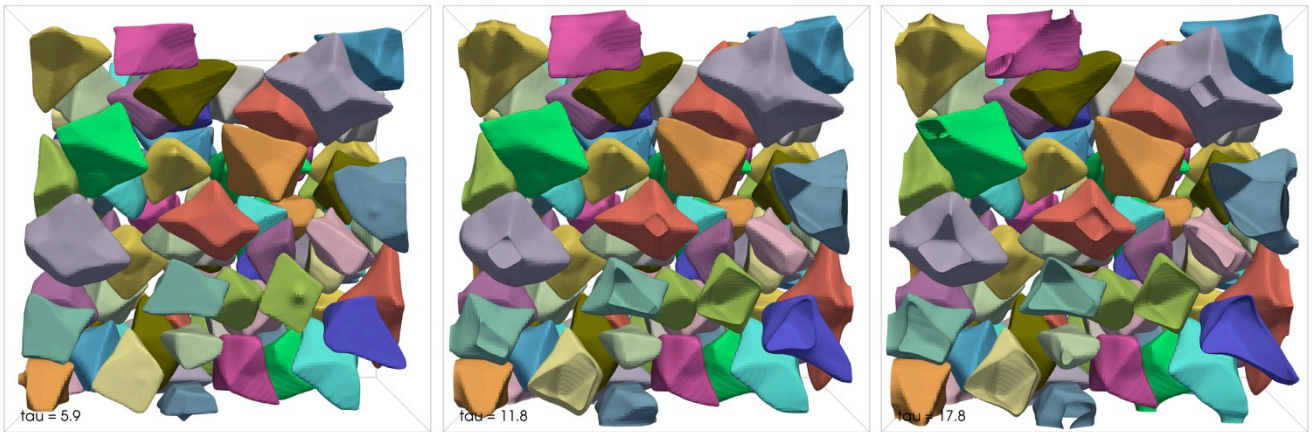
(a) 27 grains in a cubic enclosure of volume $(60\,l_{\mathrm{diff}})^3$: $N_V^{\mathrm{ldiff}} = 1.25 \cdot 10^{-3}$ ($d_0 = 22\,l_{\mathrm{diff}}$).

(b) 27 grains in a cubic enclosure of volume $(30\,l_{\mathrm{diff}})^3$: $N_V^{\mathrm{ldiff}} = 10^{-3}$ ($d_0 = 11\,l_{\mathrm{diff}}$).

(c) 108 grains in a cubic enclosure of volume $(30\,l_{\mathrm{diff}})^3$: $N_V^{\mathrm{ldiff}} = 4 \cdot 10^{-3}$ ($d_0 = 7\,l_{\mathrm{diff}}$).
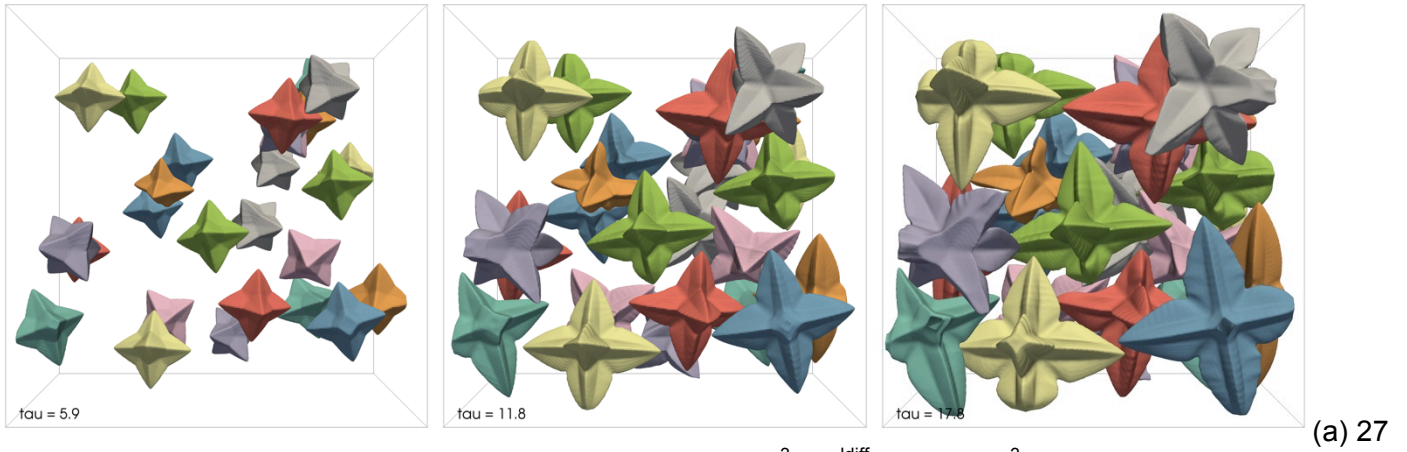
Fig. 2: Simulations of randomly distributed and oriented grains growing isothermally in a cubic enclosure at an initial supersaturation of $\Omega_0 = 0.05$ and at three different dimensionless grain densities N_V^{ldiff} (or three different mean grain distances d_0).

In a volume-averaged model such an overlap of diffusion fields is represented by a decrease of the average solute gradients at the grain envelopes. These are approximated by the difference of the concentration of the liquid at the envelope, C_l^*, and the average concentration of the extradendritic liquid, $\langle C_l \rangle^e$, divided by a diffusion length, δ_l. The evolution of the average concentration of the extradendritic liquid is given by an averaged conservation equation of the following form:

$$\frac{\partial(g_e \langle C_l \rangle^e)}{\partial t} = C_l^* \frac{\partial g_e}{\partial t} + D_l S_{V,env} \frac{C_l^* - \langle C_l \rangle^e}{\delta_l} \, , \tag{1}$$

where g_e is the volume fraction of the extradendritic liquid, $S_{V,env}$ is the the specific surface area of the envelopes per unit volume of the REV, and D_l is the diffusion coefficient. If we assume iso-thermal conditions, where C_l^* is constant, and introduce the average supersaturation of the extra-dendritic liquid, $\langle \Omega_l \rangle^e = (C_l^* - \langle C_l \rangle^e)/[(1-k) C_l^*]$, as a dimensionless concentration, Eq. (1) is rewritten as:

$$\frac{\partial(g_e \langle \Omega_l \rangle^e)}{\partial t} = -D_l S_{V,env} \frac{\langle \Omega_l \rangle^e}{\delta_l} \, , \tag{2}$$

where k is the equilibrium partition coefficient. In macroscopic volume-averaged models the evolution of the volume fraction of the extradendritic liquid, g_e, directly depends on the average supersaturation $\langle \Omega_l \rangle^e$. $S_{V,env}$ and δ_l are parameters essential for an accurate representation of the envelope growth kinetics. Both are usually modeled by simplistic analytical or empirical relations. Now they can be determined directly by averaging of the mesoscopic simulations, which represent the phenomena at the scale of the macroscopic REV in detail. The challenge is to find general relations, valid in a wide range of solidification conditions.

Such an attempt for the extreme situation of isothermal growth is illustrated in Figs. 3–4. The averaging was made with the simulations shown in Fig. 2 and with an additional set of simulations performed for an initial supersaturation of $\Omega_0 = 0.15$ and with all other parameters kept identical. Fig. 3 shows the evolution of the average supersaturation of the extradendritic liquid, $\langle \Omega_l \rangle^e$, and of the envelope fraction ($g_{env} = 1 - g_e$) with time. Note that the envelopes stop growing when $\langle \Omega_l \rangle^e$ becomes zero. We can see that with a proper choice of scalings, a generalized evolution can be obtained that depends neither on the initial supersaturation nor on the grain density. The time evolutions of both the supersaturation and the envelope fraction are scaled with a time scale of $D_l^{-1} l_{diff}^2 (N_V^{ldiff})^{-2/3}$, which is proportional to the diffusion time across the mean distance between grains, d_0^2/D_l. Fig. 4 shows the evolution of the dimensionless averaged diffusion length scaled by the tip diffusion length, δ_l/l_{diff}, and of the dimensionless specific surface of the envelopes scaled by the mean grain distance, $S_{V,env} l_{diff} (N_V^{ldiff})^{-1/3}$. Both are best characterized using time scales of $l_{diff} V_{LGK}^{-1}$ and $l_{diff} V_{LGK}^{-1} (N_V^{ldiff})^{-1/3} \sim d_0/V_{LGK}$, respectively. The first of these time scales is the time needed for a primary tip to traverse the diffusion layer in front of the tip and the second is proportional to the time needed to traverse the mean distance between the grains.
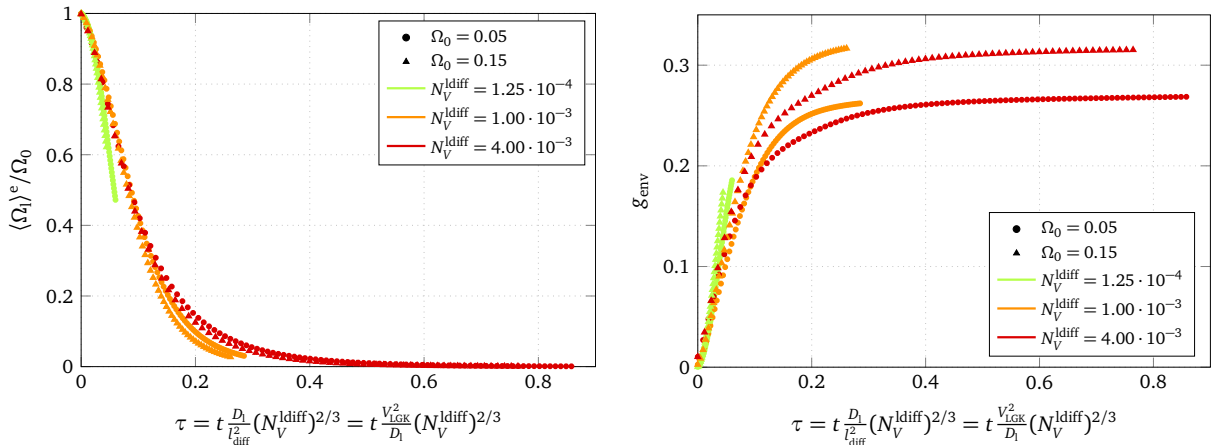

Fig. 3: Left: Evolution of the supersaturation of the extradendritic liquid. Right: Evolution of the envelope volume fraction over the dimensionless time. Both are presented in terms of dimensionless time, scaled by the characteristic diffusion time across the mean distance between grains: $D_l^{-1} l_{diff}^2 (N_V^{ldiff})^{-2/3} \sim d_0^2/D_l$.
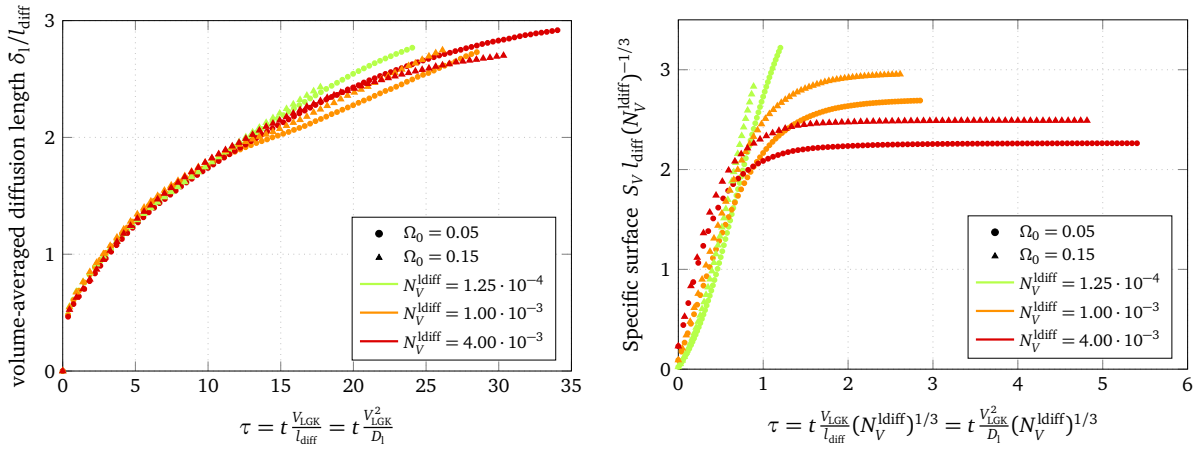
Fig. 4: Left: Evolution of the dimensionless volume-averaged diffusion length over the dimensionless time scaled by $l_{\text{diff}} V_{\text{LGK}}^{-1}$. Right: Evolution of the dimensionless specific envelope surface area over the dimensionless time scaled by $l_{\text{diff}} V_{\text{LGK}}^{-1} (N_V^{\text{ldiff}})^{-1/3} \sim d_0/V_{\text{LGK}}$.

4. CONCLUSION

We used the mesoscopic envelope model of solidification to simulate the growth of large ensembles of equiaxed grains in the presence of solutal interactions. The configurations ranged from weakly to strongly interacting. We calculated representative volume-averaged quantities for the simulated ensembles in order to extract parameters that can be used in macroscopic models. We have shown examples of the temporal evolution of the volume-averaged envelope surface area and of the volume-averaged diffusion length in the liquid at the envelope surface. With these examples we have shown that the proper choice of scalings can lead to generalized correlations that can be implemented in volume-averaged multiscale models of processes, which are used at the industrial scale. This work should be extended to more generally applicable solidification conditions that account for heat extraction from the REV and for convection.
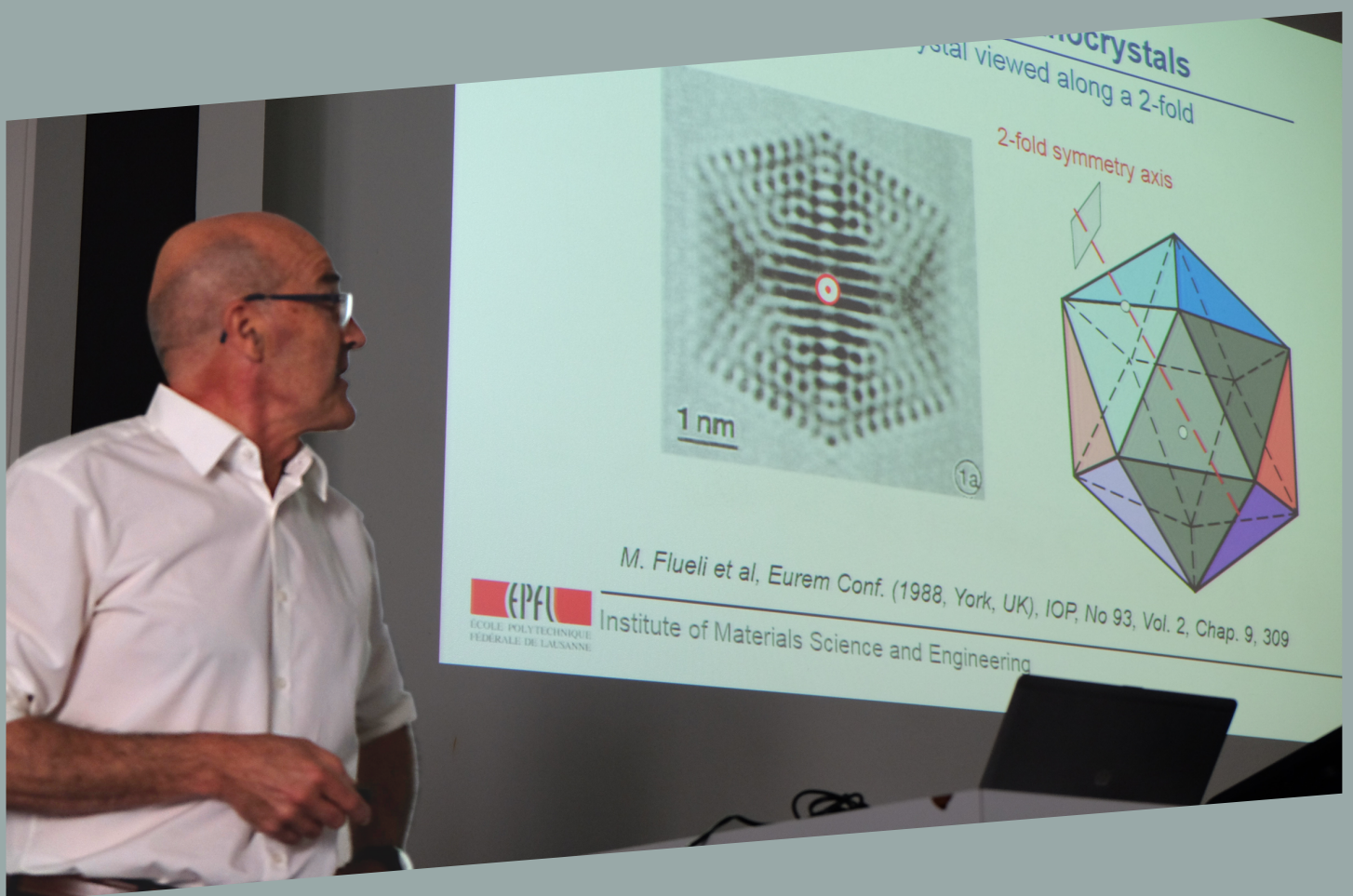
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REFERENCES

1. M. Rappaz, C.-A. Gandin, Acta Metall. Mater. **41**, 1993, 345.

2. I. Steinbach, C. Beckermann, B. Kauerauf, Q. Li, J. Guo, Acta Mater. **47**, 1999, 971.

3. I. Steinbach, H.-J. Diepers, C. Beckermann, J. Cryst. Growth **275**, 2005, 624.

4. Y. Souhar, V.F. De Felice, C. Beckermann, H. Combeau, M. Založnik, Comp. Mater. Sci. **112**, 2016, 304.

5. P. Delaleau, C. Beckermann, R.H. Mathiesen, L. Arnberg, ISIJ Int. **50**, 2010, 1886.

6. M. Založnik, A. Viardin, Y. Souhar, H. Combeau, M. Apel, IOP Conf. Ser.: Mater. Sci. Eng. **84**, 2015, 012074.

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M. Flueli et al, Eurem Conf. (1988, York, UK), IOP, No 93, Vol. 2, Chap. 9, 309

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