A phase field formulation of microstructure evolution induced by laser-based additive manufacturing with atomic defect generation

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Abstract. A phase field formulation of microstructure evolution during laser powder-bed additive manufacturing process is presented taking into account coupled heat transfer, stress effects and atomic defects (vacancies and interstitials) generation at the moving liquid-solid interface. A kinetic equation for the phase field coupled to the temperature, the concentration of atomic defects, and the elastic displacement fields is derived based on first and second laws of thermodynamics. The phenomenon of flexural instability with the PD clustering (formation of micropores and dislocation loops) and its effect on the exfoliation of deposited layers on a substrate are also discussed.

1. Introduction

Selective laser melting (SLM) is a popular powder-based additive manufacturing (AM) process for directly manufacturing of fully-dense metallic components. Nowadays, SLM is widely used in aerospace, biomedical, energy, and automotive industries [1, 2]. In powder-bed technology, parts are manufactured layer by layer, using a source of thermal energy to fuse the different layers together. In powder-bed technology, parts are manufactured layer by layer, using a source of thermal energy to fuse the different layers together. Laser powder bed fusion process has many parameters (power, scan velocity, layer thickness, etc.), that in combination with material properties and environmental conditions influence quality of fabricated parts. With more use, more needs and requirements are set to products fabricated by AM process. Ideally, AM parts should be at least equivalent, or preferably better quality than conventionally fabricated parts. One of the major problems that should be addressed is how to improve and control quality of as-built part and define what significantly influence the quality of a part.

Mechanical stresses and defect generation play an essential role in the AM process. Manufacturing defects and their effects on the quality and performance of AM parts are the most difficult issues. It is essential to understand the defect types, their formation mechanisms, and the detection methodologies for mechanical properties evaluation and quality control. The tasks of the process to reduce them are not yet resolved. In general, these effects are associated both with the process of melting the powder material (gas porosity) and solidification of the melt. In the first case, the significant effects affecting the formation of defects (pore defects) are the beam power density distribution, the surface tension, the Marangoni convection and the recoil pressure [3, 4]. In the second case the micropore formation is due to atomic point defects (PD) (vacancies and self-interstitials), formed by fluctuation at the solid site of the solid-liquid interface and their clustering in the process of diffusion.

Experimentally it is very difficult to define those parameters and their combinations, which have the most impact on mechanical and physical properties of the product. SLM is an inherently multi scale, multi physics process and calls for an approach using multiple coupled models. Existing modeling tools used to study laser processing of materials are currently being actively extended to AM modeling. There are many different approaches to the modeling of the thermal history and resulting profiles of parts manufactured by AM processes. Most of the existing studies utilize numerical methods, due to the complexity of the phenomena that take place [5-7]. However, multiscale models of solidification are needed, which will include the evolution of morphology and growth of various microstructures (grain growth, dendrites, etc.).

One of the important tasks is the quantitative inclusion of elastic effects in the model of the microstructure evolution during SLM. This is of general scientific interest in applications in which elastic fields act as a stable driving force for phase transformations (FP) or as a basic field for consistently modeling such processes as the generation and motion of non-equilibrium PDs, plasticity and others, accompanying the rapid solidification of the melt. PDs lead to local changes in interatomic distances and, consequently, to lattice distortions. In the process of cooling, PDs can migrate either due to a chemical potential gradient or elastic interaction, or to be trapped by other defects or so-called absorbers, such as dislocations, grain boundaries. The density and stability of the absorber will determine the accumulation of mobile PDs created at the liquid-solid interface, which affects the stability of the phase and/or structure and the kinetics of the microstructure development and properties of the material. The residual stresses and distortions, which are caused by the non-homogenous thermal phenomena (heating and cooling) and the PD generation that take place in AM, deteriorate the mechanical properties and the dimensional accuracy of the parts.

In the present contribution a physically thermodynamically consistent phase field model proposed by Wang et al. [8] is extended to describe the microstructure evolution during additive SLM process taking into account the coupled processes of heat transfer, stress effects and PDs generation on liquid-solid interface. Constitutive relations are derived on the basis of a single entropy functional and the principle of entropy production positiveness. The application of this principle allows obtaining consistent evolutionary equations for the phase field coupled with the fields of temperature, PD concentration and atomic elastic displacements for non-isothermal conditions of crystallization. Some applications of the developed coupled model of defect formation during solidification are considered. Diffusion-flexural instability with the formation of PD clusters (micropores and dislocation loops) and its effect on the exfoliation of deposited thin layers on a substrate are also discussed.

2. Formulation of the problem

Microstructure evolution during SLM process has negligible effect on heat transfer and temperature distribution in the build, while the heat transfer is mainly affected by the heat conductivity of the materials, as well as the AM processing parameters such as laser power, laser scan speed, beam diameter, powder feed rate et al. With these assumptions, the microstructure evolution during SLM can be decoupled into two sub models on different length scales: (i) the macroscopic thermo-hydrodynamic model to obtain the temperature and fluid velocity distributions and thermal history in the build during the whole SLM; (ii) the phase-field model for microstructure evolution during solidification at the SLM process.

We assume that the second phase can have a different lattice parameter from the mother phase, and therefore elastic stress is generated. It is also assumed that the generation of PDs on liquid-solid interface occurs. Within the phase field conception, the state of considered system at time t is defined by the five field variables: the temperature field $T(\mathbf{r},t)$, the concentration of PDs ($n(\mathbf{r},t)$), the atomic displacement field ($\mathbf{u}(\mathbf{r},t)$) representing the mechanical motion, and the phase field $\phi(\mathbf{r},t)$ for microstructure evolution. The order parameter (ϕ) is defined as 0 in liquid and 1 in solid, and smoothly varies over an interface of a certain width δ (δ has to be small compared to the microstructure length scale of interest). We denote by $\mu(\mathbf{r},t)$, $\eta(\mathbf{r},t)$ and $e(\mathbf{r},t)$ the diffusion potential of the PDs, the entropy and internal energy densities (per unit volume), respectively.

The balance laws for the energy and PDs concentration can be written as

$$\dot{e} = -\nabla \cdot \mathbf{j}^{(e)} - \nabla \cdot \left(\mu_v \mathbf{j}_v^{(n)} \right) - \nabla \cdot \left(\mu_i \mathbf{j}_i^{(n)} \right) + \boldsymbol{\sigma}\dot{\boldsymbol{\varepsilon}}, \tag{1}$$

$$\dot{n}_v = -\nabla \cdot \mathbf{j}_v^{(n)} + Q_v\left(T,\phi\right) - R_v\left(n_v,n_i,T\right), \tag{2}$$

$$\dot{n}_i = -\nabla \cdot \mathbf{j}_i^{(n)} + Q_i\left(T,\phi\right) - R_i\left(n_v,n_i,T\right), \tag{3}$$

where $\mathbf{j}^{(e)}$ is the energy flux, $\mathbf{j}_v^{(n)}$ and $\mathbf{j}_v^{(n)}$ the vacancies and self-interstitials fluxes, respectively, μ_i and μ_i, the diffusion potentials of PDs, $\boldsymbol{\sigma}$ the stress tensor, $\boldsymbol{\varepsilon}$ the total strain tensor; $Q_{v,i}\left(T,\phi\right)$ the PDs generation rates on liquid-solid interface (l-s), $R_{i,v}\left(n,T\right)$ characterize the losses of PD concentration associated with their recombination. The second and third terms in (2) represent the flux of energy carried by the fluxes of PDs [8] and the last term - changes due to strain.

We restrict attention to small strains, thus the total strain tensor is given by the sum of the elastic, thermal, concentration and phase strains, $\boldsymbol{\varepsilon}^{(el)}$, $\boldsymbol{\varepsilon}^{(th)}$, $\boldsymbol{\varepsilon}^{(d)}$ and $\boldsymbol{\varepsilon}^{(tr)}$, respectively

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{(el)} + \boldsymbol{\varepsilon}^{(th)} + \boldsymbol{\varepsilon}^{(tr)} + \boldsymbol{\varepsilon}^{(d)}\left(n_i,n_v\right), \tag{4}$$

$$\boldsymbol{\varepsilon}^{(th)} = \mathbf{B}\left(T - T_{ref}\right), \quad \boldsymbol{\varepsilon}^{(d)}\left(n_v,n_i\right) = \boldsymbol{\Omega}_v\left(n_v - n_{v0}\right) + \boldsymbol{\Omega}_i\left(n_i - n_{i0}\right),$$

where the tensor $\mathbf{B} = \partial\boldsymbol{\varepsilon}/\partial T$ takes into account the strains due to thermal expansion; $\boldsymbol{\varepsilon}^{(d)}$ is the PD induced eigen-strain, the tensor $\boldsymbol{\Omega}_{i,v} = \partial\boldsymbol{\varepsilon}/\partial n_{i,v}$ scales the defect concentration changes, n_{0i} and n_{0v} are the equilibrium PDs concentrations. For the particular case of isotropy: $\boldsymbol{\Omega} = -\alpha\mathbf{I}$, $\alpha = \left(1/a\right)da/dn$, a is the lattice parameter and $\mathbf{I}$ is the second order identity tensor); $\boldsymbol{\varepsilon}^{(tr)}$ is the strain generated from the difference in the volumes of phases l and s. For the isotropic case $\boldsymbol{\varepsilon}^{(tr)} = \chi_0\mathbf{I}$. The transformation expansion coefficient χ_0 is expressed by the formula obtained by converting the rate of volumetric change into a linear expansion coefficient $\chi_0 \approx \left(v_s - v_l\right)/3v_l$. The total strain is given by $\varepsilon_{ik} = 1/2\left(\nabla_i u_k + \nabla_k u_i\right)$.

The dissipation inequality is given by

$$\dot{\eta} \geq -\nabla \cdot \left(T^{-1}\mathbf{j}^{(e)}\right) - \alpha_\phi^2\dot{\phi}\nabla^2\phi. \tag{5}$$

α_ϕ^2 is a gradient-energy coefficient. With the use of (1), (2) and (3) we have from (5)

$$\alpha_\phi^2\dot{\phi}\nabla^2\phi + \boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}} - \dot{\psi} - \eta\dot{T} + \mu_v\dot{n}_v + \mu_i\dot{n}_i - \mathbf{j}_v^{(n)}\cdot\nabla\mu_v - \mathbf{j}_i^{(n)}\cdot\nabla\mu_i + T\mathbf{j}^{(e)}\cdot\nabla T^{-1} \geq 0, \tag{6}$$

where $\psi = e - T\eta$ is the Helmholtz free energy. The free energy density (ψ), the stress ($\boldsymbol{\sigma}$), and the entropy (η) can be expressed as a function of the following internal state variables characterizing the system behavior: the phase field (ϕ), the temperature field (T), the elastic strain ε_{ik}^e and PDs concentration (n_i,n_v) such that

$$\psi = \hat{\psi}\left(\boldsymbol{\Lambda}\right), \quad \sigma_{ik} = \hat{\sigma}_{ik}\left(\boldsymbol{\Lambda}\right), \quad \eta = \hat{\eta}\left(\boldsymbol{\Lambda}\right), \tag{7}$$

where $\boldsymbol{\Lambda}$ denotes the list $\boldsymbol{\Lambda} = \left(\phi,T,\varepsilon_{ik}^e,n_i,n_v\right)$. Differentiating (7)$_1$ in time, we get:

$$\dot{\psi} = \frac{\partial\hat{\psi}}{\partial T}\bigg|_{\boldsymbol{\varepsilon},\phi,n_i,n_v}\dot{T} + \frac{\partial\hat{\psi}}{\partial\boldsymbol{\varepsilon}}\bigg|_{\phi,T,n_i,n_v}\dot{\boldsymbol{\varepsilon}} + \frac{\partial\hat{\psi}}{\partial\phi}\bigg|_{\boldsymbol{\varepsilon},T,n_i,n_v}\dot{\phi} + \frac{\partial\hat{\psi}}{\partial n_i}\bigg|_{\boldsymbol{\varepsilon},T,\phi}\dot{n}_i + \frac{\partial\hat{\psi}}{\partial n_v}\bigg|_{\boldsymbol{\varepsilon},T,\phi}\dot{n}_v. \tag{8}$$

Substituting (8) into (6), we find

$$\left(\alpha_\phi^2\nabla^2\phi - \frac{\partial\hat{\psi}}{\partial\phi}\bigg|_{\boldsymbol{\varepsilon},T,n}\right)\dot{\phi} - \left(\eta + \frac{\partial\hat{\psi}}{\partial T}\bigg|_{\boldsymbol{\varepsilon},\phi,n} - \beta\mathrm{tr}\left(\boldsymbol{\sigma}\right)\right)\dot{T} - \left(\mu_v + \alpha_v\mathrm{tr}\left(\boldsymbol{\sigma}\right) - \frac{\partial\hat{\psi}}{\partial n_v}\bigg|_{\boldsymbol{\varepsilon},T,\phi}\right)\dot{n}_v$$

$$-\left(\mu_i + \alpha_i\mathrm{tr}\left(\boldsymbol{\sigma}\right) - \frac{\partial\hat{\psi}}{\partial n_i}\bigg|_{\boldsymbol{\varepsilon},T,\phi}\right)\dot{n}_i + \left(\boldsymbol{\sigma} - \frac{\partial\hat{\psi}}{\partial\boldsymbol{\varepsilon}}\bigg|_{\phi,T,n}\right):\dot{\boldsymbol{\varepsilon}} - \mathbf{j}^{(e)}\cdot\frac{\nabla T}{T} - \mathbf{j}_i^{(n)}\cdot\nabla\mu_i - \mathbf{j}_v^{(n)}\cdot\nabla\mu_v \geq 0. \tag{9}$$

If in inequality (9) we take into account that, and $\dot{T}$, $\dot{n}_v$ $\dot{n}_i$ and $\dot{\varepsilon}$ can change in an independent way, then to satisfy it at any values of $\dot{T}$, $\dot{n}_v$ $\dot{n}_i$ and $\dot{\varepsilon}$, we need to put

$$\eta = -\left(\partial\hat{\psi}/\partial T\right)\big|_{\varepsilon,\phi,n} + \beta\mathrm{tr}\left(\boldsymbol{\sigma}\right), \quad \boldsymbol{\sigma} = \left(\partial\hat{\psi}/\partial\varepsilon\right)\big|_{\phi,T,n}, \quad \mu_{v,i} = \left(\partial\hat{\psi}/\partial n_{i,v}\right)\big|_{\varepsilon,T,\phi} - \alpha_{i,v}\mathrm{tr}\left(\boldsymbol{\sigma}\right) \quad (10)$$

at

$$\left(\alpha_\phi^2\nabla^2\phi - \partial\hat{\psi}/\partial\phi\right)\dot{\phi} - T^{-1}\mathbf{j}^{(e)}\cdot\nabla T - \mathbf{j}_i^{(n)}\cdot\nabla\mu_i - \mathbf{j}_v^{(n)}\cdot\nabla\mu_v \geq 0. \quad (11)$$

From the inequality (11) it is possible to identify three dissipative processes. The first term represents the phase field dissipation, which is related to the rearrangement of atoms during the evolution of the phase fields. The second term is the heat transport caused by diffusion. The last two terms represent the dissipation caused by PDs. The positivity of entropy production can be locally assured having chosen the following relationships for the diffusional flows and the time derivatives of variables

$$\mathbf{j}^{(e)}\cdot\nabla T \leq 0, \quad \mathbf{j}^{(e)}\left(\phi,T\right) = m_e\left(\phi,T\right)\nabla T^{-1}, \quad (12)$$

$$\mathbf{j}_v^{(n)} = -m_v\left(\phi,T,n_v\right)\nabla\mu_v, \quad \mathbf{j}_i^{(n)} = -m_i\left(\phi,T,n_i\right)\nabla\mu_i, \quad (13)$$

$$m_\phi^{-1}\left(\phi,T\right)\dot{\phi} = \alpha_\phi^2\nabla^2\phi - \partial\hat{\psi}/\partial\phi, \quad (14)$$

where m_ϕ is the phase field mobility, $m_i > 0$, $m_v > 0$ and $m_e > 0$ characterize PDs diffusion and thermal conductivity, respectively.

3. Local governing equations
We assume that the total free energy density is given by

$$\psi = \psi^{(dw)} + \psi^{(th)} + \psi^{(el)} + \psi^{(ch)} \quad (15)$$

with

$$\psi^{(dw)}\left(\phi\right) = w_\psi g(\phi) = w_\psi\phi^2\left(1-\phi\right)^2,$$

$$\psi^{(th)}\left(T\right) = \Phi_l^{th}\left(T\right) + \Delta\Phi p\left(\phi\right),$$

$$\psi^{(ch)}\left(T,n\right) = \frac{N_a}{v_a}E_v^f n_v + Rv_a^{-1}\left(n_i\ln\left(n_i\right) + n_v\ln\left(n_v\right) - \left(1-n_i-n_v\right)\ln\left(1-n_i-n_v\right)\right).$$

Here $\psi^{dw}\left(\phi,T\right)$ is the double–well potential, guaranteeing that the free energy function has two local minima at $\phi = 0$ and $\phi = 1$ corresponding to the two phases of the system. w_ψ is the height of the energy barrier between phases. $\Phi_l^{(th)}\left(T\right)$ is the free-energy density of the liquid ($\Phi_l^{(th)}\left(T\right) = c\left(T-T_m\right) - cT\ln(T/T_m)$, c , the heat capacity, T_m , the melting temperature), $\Delta\Phi$, the difference between the energies of the l and s phases; $\Delta\Phi = L\left(T-T_m\right)/T_m$ (L is the latent heat of fusion); $p(\phi) = \phi^3\left(10-15\phi+6\phi^2\right)$ is the interpolation function with $p(0) = 0$ and $p(1) = 1$ for variation of many material property between solid and melt. E_v^f is the formation energy of vacancies, N_a , the Avogadro number; v_a , the molar volume; R_g , the universal gas constant.

The elastic energy density is interpolated between the two phases using a smooth function $p(\phi)$:

$$\psi^{(el)}\left(\mathbf{u},T,n_i,n_v,\phi\right) = p(\phi)\psi_s^{(el)}\left(\mathbf{u},T,n_i,n_v,\phi\right) + \left[1-p(\phi)\right]\psi_l^{(el)}\left(\mathbf{u},T,\phi\right). \quad (16)$$

The elastic energies of the s and l phases are given by

$$\psi_s^{(el)}\left(\mathbf{u},T,\phi,n_i,n_v\right) = 0.5\left(\varepsilon-\varepsilon_s^{(th)}-\varepsilon_s^{(tr)}-\varepsilon_s^{(d)}\right):\Lambda_s:\left(\varepsilon-\varepsilon_s^{(th)}-\varepsilon_s^{(tr)}-\varepsilon_s^{(d)}\right), \quad (17)$$

$$\psi_l^{(el)}\left(\mathbf{u},T,\phi\right) = 0.5\left(\varepsilon-\varepsilon_l^{(th)}-\varepsilon_l^{(tr)}\right):\Lambda_l:\left(\varepsilon-\varepsilon_l^{(th)}-\varepsilon_l^{(tr)}\right). \quad (18)$$

(Λ_l and Λ_s are constants). In (18) it is assumed that the elastic strain is equal in all the phases assumed to be present as a mixture at every point in the diffuse interface region corresponding to

Voigt/Teylor homogenization model. It should be noted that the contribution to the elastic energy due to PDs ($\boldsymbol{\varepsilon}_s^{(d)}$) is nonzero only for the solid phase.Combining (4), (16), (17) and (18) we have

$$\psi^{(el)}\left(\mathbf{u},T,\phi,n_i,n_v\right)=0.5\boldsymbol{\varepsilon}^{(el)}:\Lambda\left(\phi\right):\boldsymbol{\varepsilon}^{(el)},\tag{19}$$

where $\Lambda\left(\phi\right)=\Lambda_l+\Delta\Lambda p\left(\phi\right)$, $\Delta\Lambda=\Lambda_s-\Lambda_l$. In the case of an isotropic medium, the elastic moduli (Λ) depend only on the Lame constant (λ) and the shear elastic modulus (G) ($\Lambda_{ijkl}=\lambda\delta_{ij}\delta_{kl}+G\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)$), so that

$$\begin{aligned}\psi^{(el)}\left(\mathbf{u},T,\phi\right)=&\tfrac{1}{2}k\left(\phi\right)\left(\nabla\cdot\mathbf{u}\right)^2+G\left(\phi\right)\left(\varepsilon_{ik}-\tfrac{1}{3}\delta_{ik}\left(\nabla\cdot\mathbf{u}\right)\right)^2-3k\left(\phi\right)\left[\beta\left(\phi\right)\left(T-T_0\right)\right.\\&\left.+\alpha_i\left(\phi\right)\left(n_i-n_{i0}\right)+\alpha_v\left(\phi\right)\left(n_v-n_{v0}\right)+\chi\left(\phi\right)\right]\left(\nabla\cdot\mathbf{u}\right).\end{aligned}\tag{20}$$

In (20) $k\left(\phi\right)=k_l+p(\phi)\Delta k$ and $G\left(\phi\right)=G_sp\left(\phi\right)$ are the bulk and shear moduli of the mixture, $\Delta k=k_s-k_l$, $\lambda=k-2G/3$ ($k_{s,l}$, the bulk moduli of the s and l phases, respectively, G_s the shear elastic modulus of the solid phase); $\beta\left(\phi\right)=\beta_l+p(\phi)\Delta\beta$ the thermal expansion coefficient of the mixture; $\beta_{s,l}$, the thermal expansion coefficients of the s and l phases; $\Delta\beta=\beta_l-\beta_s$; $\alpha\left(\phi\right)=\alpha_0 p\left(\phi\right)$, the dilatation volume of the PDs. The last term including $\chi=\chi_0\left(T\right)p\left(\phi\right)$ allows for the stresses generated because of the difference in the volumes of l and s phases. Elastic constants λ and μ are related to Young's modulus (E) and Poisson's ratio (v) via $\mu=E/2\left(1+v\right)$ and $\lambda=Ev/2\left(1+v\right)\left(1-2v\right)$.

Then, in view of (10), the entropy and diffusion potential are given by the following expressions

$$\begin{aligned}\eta=&\eta_0+c\ln\left(T/T_0\right)-w_\psi g\left(\phi\right)+Lp\left(\phi\right)+\beta\mathrm{tr}\left(\boldsymbol{\sigma}\right)-\\&Rv_a^{-1}\left(n_i\ln\left(n_i\right)+n_v\ln\left(n_v\right)-\left(1-n_i-n_v\right)\ln\left(1-n_i-n_v\right)\right)\end{aligned}\tag{21}$$

$$\mu_v=\partial\psi^{ch}/\partial n_v-\boldsymbol{\sigma}^s:\boldsymbol{\Omega}^{v,s}p\left(\phi\right),\tag{22}$$

$$\mu_i=\partial\psi^{ch}/\partial n_i-\boldsymbol{\sigma}^s:\boldsymbol{\Omega}^{i,s}p\left(\phi\right).\tag{23}$$

The expression for the elastic stress, following from (10)$_2$ and (20) has the form $\boldsymbol{\sigma}=\Lambda\left(\phi\right):\boldsymbol{\varepsilon}^{(el)}$ or

$$\begin{aligned}\sigma_{ik}=&\frac{E\left(\phi\right)}{1+v\left(\phi\right)}\left[\varepsilon_{ik}+\frac{v\left(\phi\right)}{\left(1-2v\left(\phi\right)\right)}\delta_{ik}\nabla\cdot\mathbf{u}\right]-3k\left(\phi\right)\delta_{ik}\left[\beta\left(\phi\right)\left(T-T_0\right)+\right.\\&\left.+\alpha_i\left(\phi\right)\left(n_i-n_{i0}\right)+\alpha_v\left(\phi\right)\left(n_v-n_{v0}\right)+\chi\left(\phi\right)\right].\end{aligned}\tag{24}$$

Substituting (15) into (14), we obtain the following kinetic equation for the phase field

$$\begin{aligned}m_\phi^{-1}\dot{\phi}=&\alpha_0^2 T\nabla\cdot\left(\tilde{\alpha}\nabla\phi\right)-\omega_\psi\frac{dg}{d\phi}+\left[\Delta G\left(T\right)+3k\left(\Delta\beta\left(T-T_0\right)+\right.\right.\\&\left.\left.+\Delta\alpha_i\left(n_i-n_{i0}\right)+\Delta\alpha_v\left(n_v-n_{v0}\right)+\chi_0\right)\left(\nabla\cdot\mathbf{u}\right)\right]\frac{dp}{d\phi}\\&+\left(0.5\Delta k\left(\nabla\cdot\mathbf{u}\right)^2+\mu_s\left(\varepsilon_{ik}-\tfrac{1}{3}\delta_{ik}\left(\nabla\cdot\mathbf{u}\right)\right)^2\right)\frac{dp}{d\phi}.\end{aligned}\tag{25}$$

Using the energy balance (1), as well as the constitutive relation (7)$_1$, we have the following energy equation

$$T\dot{\eta}+\frac{\partial\hat{\psi}}{\partial\phi}\dot{\phi}+\frac{\partial\hat{\psi}}{\partial n_i}\dot{n}_i+\frac{\partial\hat{\psi}}{\partial n_v}\dot{n}_v=-\nabla\cdot\mathbf{j}^{(e)}+\nabla\mu_i\cdot m_n\nabla\mu_i+\nabla\mu_v\cdot m_n\nabla\mu_v.\tag{26}$$

If in (26) to substitute the expression for $\dot{\eta}$

$$\dot{\eta}=\left(\partial\hat{\eta}/\partial T\right)\dot{T}+\left(\partial\hat{\eta}/\partial\boldsymbol{\varepsilon}^{(el)}\right)\dot{\boldsymbol{\varepsilon}}^{(el)}+\left(\partial\hat{\eta}/\partial\phi\right)\dot{\phi}+\left(\partial\hat{\eta}/\partial n_i\right)\dot{n}_i+\left(\partial\hat{\eta}/\partial n_v\right)\dot{n}_v$$

and take the designation for heat capacity $c = -T \partial^2 \hat{\psi} / \partial T^2$, then the energy conservation law takes the form of the heat equation, which takes into account the relationship between temperature, PD concentration, stress and phase field:

$$c\dot{T} = \nabla(\kappa \nabla T) - 3T\beta(\phi))\text{tr}(\dot{\sigma}) + \nabla \mu_i \cdot m_n \nabla \mu_i + \nabla \mu_v \cdot m_n \nabla \mu_v +$$

$$T\left(\frac{\partial \mu_v}{\partial T}\dot{n}_v + \frac{\partial \mu_i}{\partial T}\dot{n}_i\right) - \left(\frac{dp}{d\phi}L + Tw_\phi \frac{dg}{d\phi}\right)\dot{\phi}. \tag{27}$$

Here we used the total heat capacity $c = c_l + (c_s - c_l)p(\phi)$ (c_l and c_s are the heat capacity for the melt and solid, respectively) and the thermal conductivity $\kappa = m_e T^{-2} = \kappa_l + (\kappa_s - \kappa_l)p(\phi)$ (κ_l and κ_s are thermal conductivity for the melt and solid, which are measured experimentally). In (27) thermo-mechanical coupling term $3T\beta(\phi))\text{tr}(\dot{\sigma})$ in the right-hand side is responsible for the Gough-Joule effects, i.e. when strain lead to structural heating and the coupling terms from third to sixth arise due to dissipative effects caused by the PD concentration diffusion.

The PDs fluxes are expressed as

$$\mathbf{j}^{(k)} = -D_k \nabla n_k + \frac{1}{3}\frac{D_k}{k_B T}n_k(1-n_k)\nabla\left[\sigma^s : \Omega^{k,s}p(\phi)\right] \tag{28}$$

($D_k = k_B T m_n(T)/n_k(1-n_k)$ the diffusivity of PDs, $k = \{i, v\}$). Combining this expression with (2) and (3), we obtain the equations of the kinetics of the PD subsystem in the form

$$\dot{n}_v = \nabla\left(D_v(n_v)\nabla n_v\right) + \frac{1}{3}\frac{D_v}{k_B T}\nabla\left(n_v(1-n_v)\nabla\left(p(\phi)\sigma^s : \Omega^{v,s}\right)\right)$$

$$- n_v^*(T)6\phi(1-\phi)\dot{\phi} - \tau_v^{-1}n_v - R_{v,i}, \tag{29}$$

$$\dot{n}_i = \nabla\left(D_i(n_i)\nabla n_i\right) + \frac{1}{3}\frac{D_i}{k_B T}\nabla\left(n_i(1-n_i)\nabla\left(p(\phi)\sigma^s : \Omega^{i,s}\right)\right)$$

$$- n_i^*(T)6\phi(1-\phi)\dot{\phi} - \tau_i^{-1}n_i - R_{v,i}, \quad (\phi \neq 0) \tag{30}$$

with $R_{v,i} = 4\pi(D_i + D_v)a\exp\left(-E_{v,i}^{(f)}/T\right)\left(n_v n_i - n_v^{(eq)}n_i^{(eq)}\right)$ and $n_{i,v} \equiv 0$, $(\phi = 0)$, where, n_i, D_i are the concentration and the diffusion coefficient of interstitial atoms, respectively. $\tau_{v,i}^{-1}$ are the recombination rates of PDs on sinks. The last term on the right-hand side (29) and (30) takes into account the effects of mutual recombination of PDs.

The elastic field can be obtained in terms of the phase field using the local equilibrium condition. Ignoring inertia and body forces, conservation of linear momentum yields: $\nabla \cdot \sigma_{ik} = 0$ or

$$\nabla_i\left[k(\phi)(\nabla \cdot \mathbf{u}) - 3k\left(\alpha_i(\phi)n_i + \alpha_v(\phi)n_v + \beta(\phi)T + \chi_0 p(\phi)\right)\right] +$$

$$+ 2\nabla_k\left[G(\phi)\left(\varepsilon_{ik} - \tfrac{1}{3}\delta_{ik}\nabla \cdot \mathbf{u}\right)\right] = 0. \tag{31}$$

Eqs. (25), (27) and (29)-(31) constitute a closed system of equations of the PFM for the microstructure evolution during SLM process. The microstructure evolution is determined by the thermal history of the materials, which is result of laser energy absorption by the powder particles and substrate, heat and mass transfer within the build part and heat losses. To describe the effects of temperature and fluid velocity distributions and thermal history on the microstructure growth kinetics the developed theory should added to the macroscale model [10] of dynamic processes accompanied SLM. The model of the processes at the macroscopic level considered by [10] takes into account the interaction of laser radiation with the powder particles, the evolution of the free surface (the interface between the melt-gas phase), hydrodynamics and heat and mass transfer in the fusion zone. The energy equation of the multiphase mixture takes into account convective and conductive flows, as well as the latent heat release accompanying the phase transition. The dynamics of convective currents is modeled with the use of a complete system of equations for the continuity of a multiphase mixture and the motion of a multiphase mixture with allowance for the action of capillary and thermo-capillary forces on the free

surface. For tracking the free surface of the melt, a volume of fluid method can be used. At this structural level the processes in a scale of the condensed system in the whole are considered and processes in two-phase region, where the formation of the microstructure takes place are not included. Thus, macromodel predicts the temperature field coupled with the convection flow velocity, and changes in the form of the free surface in the process of SLM

The temperature distributions found from the the microscopic model can be used as boundary and initial conditions for solving the problem of the evolution of the microstructure. It allows investigating the influence on the microstructure formation of both the SLM parameters and the parameters of microprocesses such as diffusion of heat and defects, lattice dilatation, strain-induced drift of PDs. etc. In addition, based on it, instability phenomena accompanying the process of melt solidification can be studied. In particular, at high PDs concentration, due to the defect-deformation positive feedback, both periodic distributions of defects and their localized states - stable PDs clusters can occur.

4. Diffusion-elastic instability of elastic layers

One of the most important manifestations of the cooperative defect-deformation interaction during microstructure evolution is the phenomenon of clusterization of similar atomic PDs, with the formation of micro- and nanometer-clusters. The clustering process occurs due to instability of the homogeneous distribution of carriers interacting through the elastic deformation fields created by them (the diffusion-elastic instability of the (DEI). DEI occurs when the average carrier concentration exceeds a certain critical value. With DEI, fluctuations in the concentration of disorder carriers, being elastic inclusions, create a deformation of the elastic continuum, which in turn leads to the appearance of deformation-induced drift of the carriers. Due to the redistribution of carriers, forces appear that are proportional to the gradient of their concentration (∇n) and directed in the compression region (for v -defects with dilatation volume $\alpha^{(v)} < 0$), and in the stretching region (for i-defects with $\alpha^{(i)} > 0$). When a certain critical concentration n_{cr} is exceeded, these forces increase small fluctuations of carrier concentrations, and an instability of the concentration field (as well as the field of elastic deformation of the medium) arises.

With the use of (25), the expression for the total flux of defects becomes

$$\mathbf{j}^{(n)} = \mathbf{j}_D + \mathbf{j}_{dr} = -D_v \left(1 - nk\alpha^{(j)2} / k_B T\right)\nabla n = D_{eff}\left(n\right)\nabla n . \tag{32}$$

Inclusion of the elastic deformation effects gives rise to an additional term in the above expression ($\mathbf{j}_{dr}$) and it represents the flux opposite to the usual diffusion ($\mathbf{j}_D$) in a system with defects of the same type ($\alpha^{(j)2} > 0$ for $\alpha^{(j)} > 0$ and $\alpha^{(j)} < 0$). In the case of PDs of different types ($\alpha^{(i)}\alpha^{(v)} < 0$) the additional flux has the same direction as the diffusion flux. The PDs with $\alpha^{(j)} < 0$, for example, vacancies, compress the lattice (reduce the volume) and the compressed regions attract PDs with $\alpha^{(j)} < 0$ and repel those with $\alpha^{(j)} > 0$.

The quantitative conditions for the appearance of clusters in a system of PDs of the same type, for example, vacancies, can be found by substitution of Eq. (32) into continuity equation $\dot{n} + \nabla \cdot \mathbf{j}^{(n)} = Q_0 - \tau^{-1}n$ ($Q_0 = const$) and linearization of the latter in the vicinity of the homogeneous solution ($n_0 = Q_0\tau$). The DEI increment (Γ) is then

$$\Gamma\left(q\right) = -Dq^2\left(1 - n_0 k\alpha^2 / k_B T\right) - \tau^{-1}$$

(q is the wave number). It therefore follows that the system is unstable if

$$Q_0 > Q_{cr} = k_B T / k\tau^{-1}\alpha^2 , \quad q^2 > q_{cr}^2 = k_B T_0 / \tau\left(k\alpha^2 n_0 - k_B T_0\right). \tag{33}$$

Physically, the fulfillment of conditions (33) is equivalent to a local change in the sign of the effective diffusion coefficient of the PDs: $D_{eff} = D\left(1 - \alpha^2 k n_0 / k_B T_0\right)$. This means that the homogeneous distribution of PDs, starting from a certain critical rate of their formation, which is determined by temperature, dilatation volume, elastic modulus, and density of recombination centers, becomes unstable. A strain-induced current arises, leading to an increase in the areas of compression (for v -

defects) or tension (for i-defects) of the concentration of defects, to their satiation and the formation of the corresponding clusters. The second inequality in (33) imposes a restriction on the spatial scale of inhomogeneities. If we accept that, $\alpha \approx 10^{-23}\,\text{cm}^3$, $k = 5.10^{11}\,\text{erg cm}^{-3}$ then $Q_{cr} = 10^{-2}\,\text{s}^{-1}$.

In the case of thin layers (coatings) on the substrate, the role of the strain field is played the bending coordinate $\xi(x,y)$, which characterizes the displacement of the points of the median plane of the film along z-axis (the z - axis is perpendicular to the layer plane, the plane $z = 0$ coincides with the midplane of the layer). Using the relationship between the layer strain $\boldsymbol{\varepsilon}_f = (\nabla \mathbf{u})_f$ and the bending coordinate: $\varepsilon_f = \nu(z - ^h\!/_2)\Delta\xi$, $\nu = (1 - 2\sigma_p)/(1 - \sigma_p)$ (h - layer thickness) for the strain-induced current of PDs along the layer surface, we have: $j_{dr} = -n_0 D\left(\nu\vartheta\,h/2k_B T\right)\nabla(\Delta\xi)$.

The equation for bending deformation will be obtained if we take into account that from the PD subsystem side (along z) there acts a force bending the film

$$\frac{h^2 c_f^2}{12}\Delta^2\xi = -\nu\vartheta_d\left(\rho h\right)^{-1}\int_{-h/2}^{h/2}(z - h/2)\Delta n\,dz,$$

where $c_f^2 = E_f/\rho_f\left(1 - \sigma_f^2\right)$ is the layer rigidity, $\vartheta_d = \kappa\alpha$ the deformation potential of the defect. The corresponding dispersion equation of DEI is

$$\Gamma(q) = Dq^2\left(n_0\frac{\vartheta_d^2\nu^2}{2\rho_f k_B T c_f^2} - 1\right) - \tau^{-1}.$$

For the occurrence of DEI it is necessary that the PDs concentration exceeds a critical value $n_{cr} = 2\rho_f k_B T_0 c_f^2/\vartheta_d^2\nu^2$. The inhomogeneous flexural strain, interacting with the vacancies produced as the film grows, produces under certain conditions a vacancy drift directed counter to the diffusion in the vacancy system. In this case the compression regions attract the vacancies, while the tension regions repel them. Becoming localized in the compression region, the vacancies themselves deform the film, enhancing thereby the initial fluctuations of the strain. The ensuing instability leads to formation, in the vacancy localization regions, of a high supersaturation sufficient for pore nuclei to appear and grow. In result, the adhesion of a layer to its substrate becomes weaker at the positions of such pore clusters and peeling off of the SLM layer can be observed.

5. Conclusions

To ensure the required mechanical and physical properties of SLM parts, it is necessary to conduct a thorough joint study of the processes of heat propagation, formation and growth of various defects and deformation using physical and mathematical models. Most microdefects are formed during crystal growth as a result of diffusion agglomeration of PDs. In this work, a coupled phase field temperature-diffusion-stress formulation for microstructure evolution during SLM has been presented with PD generation on liquid-solid interface. The model has been developed in a formal thermodynamic setting, with entropy functional instead of a Helmholtz free energy functional associated with microstructural non-isothermal processes, the postulation of energy balance and demonstration that the classical entropy inequality is satisfied. Various couplings terms introduce dependencies between different processes. The governing equations that follow from the fundamental balance laws involve the phase variable, the atomic displacement field, and the defect concentration field, with significant couplings between all equations. The model includes concentration-dependent eigen-strain, strain due to PT, strain dependency on PT and local mechanical equilibrium conditions.

The dynamics equations of the of the PDs subsystem take into account the diffusion (ordinary and stress-induced drift) of the PDs concentration, their recombination on neutral absorbers. The energy transfer equation includes contributions to the energy balance associated with dissipative effects generated by a change in the PDs concentration, as well as by the generation of latent heat due to phase changes. Some applications of the proposed coupled model of defect evolution have been discussed. The thermodynamically consistent approach used to derive control equations is characteristic not only for the solidification during SLM process, but covers a wide class of problems

(laser heating of solids, laser synthesis of thin films, etc.), in which thermal conductivity, diffusion of defects, and elastic effects are related.

The microstructure evolution during SLM is determined by the thermal history of parts, which is result of laser beam energy absorption by the powder particles and substrate, heat and mass transfer within the build part and heat losses. The resultant inhomogeneous temperature distribution and thermal history from the macroscopic thermo-hydrodynamic model can be used as the initial and boundary conditions for defect diffusion, which influences grain growth during SLM. Linking of microstructure evolution by considering the relationship of micro - and macroparameters, including laser and powder parameters such as laser power, scanning probe size and scan velocity will lead to a better understanding of different aspects of the microstructure evolution during the SLM.

6. References

[1]   Mani, M. A review on measurement science needs for real-time control of additive manufacturing metal powder bed fusion processes / M. Mani, B.M. Lane, M.A. Donmez, S.C. Feng, S.P. Moylan // Int. J. Production Research. – 2017. – Vol. 55(5). – P. 1400-1418.

[2]   Wong, M. Selective laser melting of heat transfer devices / M. Wong, S. Tsopanos, C. Sutcliffe and L. Owen // Rapid Prototyping Journal. – 2007. – Vol. 13(5). – P. 291-297. DOI: 10.1108/13552540710824797.

[3]   Khairallah, S.A. Laser powder-bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones / S.A. Khairallah, A.T. Anderson, A. Rubenchik, W.E. King // Acta Materialia. – 2016. – Vol. 108. – P. 36-45.

[4]   Xia, M. Selective laser melting 3D printing of Ni-based superalloy: understanding thermodynamic mechanisms / M. Xia, D. Gu, G. Yu, D. Dai, H. Chen, Q. Shi // Sci. Bull. – 2016. – Vol. 61(13). – P. 1013-1022. DOI: 10.1007/s11434-016-1098-7.

[5]   Li, Y. Parametric analysis of thermal behavior during selective laser melting additive manufacturingof aluminum alloy powder / Y. Li, D. Gu // Mater Des. – 2014. – Vol. 63. – P. 856-867.

[6]   Zang, D.Q. Select laser melting of W–Ni–Fe powders: simulation and experimental study / D.Q. Zang, Q.Z. Cai // Int. J. of Advanced Manufacturing Technology. – 2010. – Vol. 51(5-8). – P. 649-658.

[7]   Panwisawas, C. Mesoscale modelling of selective laser melting: Thermal fluid dynamics and microstructural evolution / C. Panwisawas, Ch. Qiu, M.J. Anderson // Computational Materials Science. – 2017. – Vol. 126. – P. 479-490.

[8]   Wang, S.-L. Thermodynamically-consistent phase-field models for solidification / S.-L. Wang, R.F. Sekerka, A.A. Wheeler // Phys. D. – 1993. – Vol. 69. – P. 189.

[9]   Gurtin, M.E. Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a microforce balance // Physica D. – 1996. – Vol. 92(3-4). – P. 178-192. DOI: 10.1016/0167-2789(95)00173-5.

[10]   Mirzade, F.Kh. On model of microstructure formation during selective laser melting of metal powder bed / F.Kh. Mirzade, A.V. Dubrov // CEUR Workshop Proc. – 2017. – Vol. 1900. – P. 108-116.