Chapter 1

Introduction and Literature Review

1.1. High temperature structural materials and micromechanical deformation modelling

During service, high temperature structural materials are exposed to the elevated temperature under the load for prolonged time. It is very difficult to withstand at this severe conditions for any simple material. Thus, creep resistance and excellent oxidation resistance are the prerequisites for materials going to be used in these severe conditions (at high temperature under load). For example, super alloy Inconel 718 [1-7] is used for the fabricating the hot parts of aero engines. Similarly, RAFM tempered martensitic steel [8-15] and 316 LN steel [16-22] are observed to be the prominent candidates for power plants components operated at high-pressure and high temperature.

Manufacturing the defect free components from high temperature materials needs a better understanding of material flow response, as they are processed through the routes like rolling, forging and extrusion. Optimized processing condition is required to control the microstructure during thermomechanical processing. Since, controlling the microstructure during processing enables the achievement of desirable mechanical properties and offers valuable insights for designing new alloys also.

Once the material is loaded in form of a structural component at high temperatures, there will be continuous degradation in microstructure, due to substructure modification in terms of coarsening of precipitates, dislocation density change and creep cavity formation. Thus the components exposed to such conditions fail after some time and the prediction of the safe life is one of the major concern to avoid any unprecedented accident.

Examining the flow and creep response of the metals and alloys employing constitutive models pertaining to microstructural-based input parameters and variables helps in understanding deformation characteristics that, in turn, influence the response of the material during creep and metal forming operations. In this direction, two approaches are often used to model the deformation behavior: a) first one is empirical based and does not deal with the physics of the deformation and b) the second approach is physically based and it is more close to reality of deformation and has a definite relation with microstructure evolution. While addressing the flow stress response or creep many empirical and physical based models have been developed. Therefore, the subsequent subchapters include a literature review related to models developed in the past decades. Furthermore, based on the literature gap in the existing models, subsequent chapters include the model development to study the flow stress response and creep for the aforementioned high-temperature materials.

1.2. Empirical based flow stress models

1.2.1. Johnson–Cook Model, 1983

Johnson–Cook [23] developed the empirical based model to study the flow stress response of OFHC Cu, Armco Iron and 4340 Steel. The flow stress is estimated through the following constitutive equation,

$$\sigma_{flow} = (A + B\varepsilon^n)\,(1 + Cln\dot{\varepsilon}^*)(1 - T^{*m}) \tag{1.1}$$

where A, B, C and m are the material constants, $\dot{\varepsilon}^{*} = \dot{\varepsilon}/\dot{\varepsilon_{ref}}$ is the dimensionless strain rate, where $\dot{\varepsilon}$ is the strain rate and $\dot{\varepsilon_{ref}}$ is the reference strain rate and T^{*m} is the homologous temperature.

1.2.2. Zerilli–Armstrong Model, 1987

Zerilli–Armstrong [24] proposed a model to study the hot deformation behavior of different BCC materials. The flow stress was estimated using the following equation,

$$\sigma = C_1 exp(-C_3 * T + C_4 T ln\dot{\varepsilon}) \tag{1.2}$$

where, C_1, C_3, C_4 are materials constant and T is temperature. Similarly, Zerilli–Armstrong[24] model also proposed the constitutive equation to study the hot deformation behavior for the different the FCC materials.

$$\sigma = C_2 \epsilon^{1/2} exp(-C_3 * T + C_4 T ln\dot{\varepsilon}) \tag{1.3}$$

1.2.3. Y.C. Lin and X. M. Chen Model, 2010

A combined model, based on Johnson–Cook and Zerilli–Armstrong [23] approach was proposed by Lin et al. [25] to study the hot deformation behavior of high strength low alloyed steel. The flow stress was estimated using the following equation,

$$\sigma = (A + B\varepsilon^{n})\ exp(-C_3 T + C_4 T ln\dot{\varepsilon}^{*}) \tag{1.4}$$

All the constants have the conventional sense.

1.3. Physics Based Flow Stress Model

Unlike the empirical-based flow stress models, which simulate the flow curves only, the physically-based flow stress models provide insights about the microstructure evolution also. In this direction several models were developed and discussed in the next subsections.

1.3.1. Y. Bergström Model, 1970

Bergström [26] proposed a model to study the stress-strain behavior of alpha iron considering the internal variables such as mobile and immobile dislocation densities. The evolution of immobile dislocation density was expressed as,

$$\frac{d\rho_i}{d\varepsilon} = U(\varepsilon) - A - \Omega\,\rho, \tag{1.5}$$

where U represents the dislocation storage and Ω represents the probability remobilization and annihilation during the interaction between mobile and immobile dislocation and assumed to be $\ll 1$ and ρ is total dislocation density composed of mobile dislocation density (ρ_m) and immobile dislocation density (ρ_i). The total flow stress response of alpha iron consists of two components: athermal stress and thermal stress, expressed as follows,

$$\sigma = \sigma_{i0} + \sigma_u \left|\frac{\dot{\varepsilon}}{Mb\rho_m}\right|^{\frac{1}{m^*}} + \alpha G b \left(\frac{U - A}{\Omega}\left(1 - e^{-\Omega\varepsilon}\right) + \rho_0 e^{-\Omega\varepsilon}\right)^{\frac{1}{2}}, \tag{1.6}$$

where σ_{i0} is the strain independent friction stress, σ_u is the effective stress corresponds to dislocation with average unit velocity, $\dot{\varepsilon}$ is strain rate, M is Taylor factor, b is the magnitude of Burgers vector, m^* is the temperature-dependent material constant, α is dislocation interaction parameter, G is room temperature shear modulus, ε is strain and ρ_0 is constant. In summary, the Bergström model [26] provides a mechanistic understanding of flow stress evolution in materials, linking dislocation density and interactions to macroscopic flow stress behavior.

1.3.2. F. Barlat et al. Model, 2002

Barlat et al. [27] proposed a model to study the stress-strain behavior and microstructure evolution of aluminum alloy during hot deformation. There were three internal variables under consideration for the model development and adopted form [28]. The internal variables include forest dislocation, mobile dislocation and mean free path of dislocation. The evolution of forest dislocation density w.r.t to shear strain is expressed as,

$$\frac{d\rho_f}{d\gamma} = \lambda_{mean} - K_2\rho_f \tag{1.7}$$

where ρ_f is forest dislocation density, λ_{mean} is the mean free path and K_2 is dynamic recovery parameter. The evolution of mean free path was expressed as,

$$\frac{d\lambda_{mean}}{d\gamma} = K_{L_m}(\lambda_{mean} - \lambda_{ms}) \tag{1.8}$$

where K_{L_m} is the saturation rate of mobile dislocation and λ_{ms} is the saturation mean free path. The evolution of mobile dislocation density w.r.t to shear strain is expressed as,

$$\frac{d\rho_m}{d\gamma} = \lambda_{ms} - \lambda_{mean} \tag{1.9}$$

The flow stress is estimated as per the Taylor hardening approach,

$$\sigma = \sigma_0 + \alpha MGb\sqrt{\rho_f} \tag{1.10}$$

Where σ_0 is short-range stress. The modelled flow curves show reasonable agreement with experimental ones with the consideration of three internal variables. It demonstrated that, class B alloy shows more strain hardening rate as compared to class A alloy. Experimental observations also confirmed that class B exhibited a higher dislocation density.

1.3.3. Y.C. Lin and D.X. Wen Model, 2014, 2016

Lin et al. [29] proposed a model to address the flow behavior and microstructure evolution during the hot deformation in the nickel based super alloy. The total flow stress is comprised of short range and long range stress and expressed as,

$$\sigma_{flow} = \underbrace{\alpha GbM\sqrt{\rho_i} + \left(-X_{drx} f_g g^{-1/2}\right)}_{long\ range\ stress} + \underbrace{0.7 g^{-0.123}\left(\dot{\varepsilon} e^{\frac{663870}{RT}}\right)^{0.09}}_{short\ \ range\ stress}, \quad (1.11)$$

where X_{drx} is recrystallization volume fraction, R is gas constant, f_g is grain size coefficient and g is grain size. Considering work hardening (WH), dynamic recovery (DRV) and dynamic recrystallization (DRX), the evolution of immobile dislocation density is expressed as,

$$\dot{\rho}_i = \frac{M}{b}\left(\frac{\sqrt{\rho_i}}{f_w} + \frac{1}{g_{avg}}\right)\dot{\varepsilon} - f_v\, \rho_i\, \dot{\varepsilon} - X_{drx} f_{drx} \rho_{i-cr}\, \dot{\varepsilon} \quad (1.12)$$

Where f_w is work hardening coefficient, g_{avg} is average grain size, f_v is dynamic recovery coefficient, f_{drx} is dynamic recrystallization coefficient and ρ_{i-cr} dislocation density in newly dynamically recrystallized grain. The dynamic recrystallizations fraction is expressed as,

$$X_{drx} = 1 - exp\left[-ln2\left(\frac{\varepsilon-\varepsilon_c}{\varepsilon_{0.5}-\varepsilon_c}\right)^{f_d}\right]; \varepsilon \geq \varepsilon_c \quad (1.13)$$

Where f_d is a material parameter. In addition to flow curves, this model [29] also predicts the evolution of grain size, and its negative influence on grain boundary strengthening has been discussed. Model [29] also addressed the impact of recrystallized grain size on the work hardening and dynamic softening.

1.3.4. X. Tang et al. Model, 2016

Tang et al. [30] proposed a model for Ni-based super alloy to understand the hot deformation behavior and total flow stress was considered to be the summation of athermal and thermal stress components as, $\sigma = \sigma_{athermal} + \sigma_{thermal}$. Athermal component considers the contribution from strain hardening and grain boundary strengthening and expressed as,

$$\sigma_{athermal} = M\alpha Gb\sqrt{\rho} + K_{HP}g^{-\frac{1}{2}} \quad (1.14)$$

Where K_{HP} is Hall-Petch parameter.The thermal stress component is associated with short-range obstacles which can be overcome by means by temperature effect and expressed as [31],

$$\sigma_{thermal} = \alpha_0 \sinh^{-1}\left(\left(\frac{\dot{\varepsilon}}{\alpha_1}\right)^{\frac{1}{n}}\right) \quad (1.15)$$

Whereas α_0 and $\alpha_1$are material constants and n is strain rate sensitivity. By considering the work hardening and dynamic recovery [32] and DRX [33], the evolution of dislocation density is expressed as,

$$\dot{\rho} = \left(k_1\sqrt{\rho} - k_2\rho\right)\dot{\varepsilon} - \frac{k_r(\rho-\rho_0)}{(1-X_{drx})^{\gamma}}\dot{X_{drx}}\ , \quad (1.16)$$

where k_1 is coefficient of work hardening and k_2 is coefficient of dynamic recovery, k_r is the materials constant and ρ_0 is the initial dislocation density. The evolution rate of dynamic recrystallization fraction is expressed as,

$$\dot{X_{drx}} = \frac{\omega_0}{T} exp\left(-\frac{Q_X}{RT}\right)\frac{Gb^2}{2}\rho\,(1-X)^{c_1}\ , \quad (1.17)$$

where ω_0, c_1 and Q_X are the material constants. The average grain size during the severe plastic deformation is estimated through rule of mixture by considering deformed grain (g_s) and dynamically recrystallized grains (g_{drx}) as,

$$g_{avg} = g_{drx}X_{drx} + g_s(1 - X_{drx}) \tag{1.18}$$

The model [30] demonstrated the impact of temperature and strain rate on thermal stress, a key component of flow stress. Additionally, it examined the different contributors of strengthening and concluded that dislocation strengthening plays the dominant role.

1.3.5. L. E. Lindgren et al. Model, 2017

Lindgren et al. [34] established the physical-based flow stress model for AISI 316L steel and total flow stress was considered to be the summation of athermal and thermal stress components as, $\sigma = \sigma_{athermal} + \sigma_{thermal}$. The athermal stress contribution due to dislocation strengthening is estimated as,

$$\sigma_{dis} = M\alpha Gb\sqrt{\rho}_i \tag{1.19}$$

The evolution rate of immobile dislocation density is expressed as,

$$\dot{\rho_i} = \dot{\rho_i}^{+} - \dot{\rho_i}^{-} \tag{1.20}$$

$$\dot{\rho_i}^{+} = \frac{M}{b}\dot{\bar{\varepsilon}^p}\left(\frac{1}{s} + \frac{1}{g}\right) \tag{1.21}$$

Where $\dot{\bar{\varepsilon}^p}$ is plastic strain rate and s is substructure size. Reduction in dislocation density can be estimated by considering the static and dynamic recovery as,

$$\dot{\rho_i}^{-} = \dot{\rho}_{sr}^{-} - \dot{\rho}_{dr}^{-} \tag{1.22}$$

Static recovery is expressed as,

$$\dot{\rho}_{sr}^{-} = c_{sr} D_v \frac{Gb^3}{k_B T}\left(p_i^2 - p_{grwn}^2\right) \tag{1.23}$$

where c_{sr} is constant, D_v is lattice diffusion coefficient, k_B is Boltzmann constant and ρ_{grwn} is dislocation density in newly formed grains. The dynamic recovery is expressed as,

$$\dot{\rho}_{dr}^{-} = \Omega \rho_i \dot{\bar{\varepsilon}}^p \tag{1.24}$$

In addition to dislocation strengthening, the athermal component also includes Hall-Petch effect and contribution due to grain boundary strengthening is estimated as,

$$\sigma_{HP} = \frac{K_{HP} G_T}{G} \frac{1}{\sqrt{g}} \tag{1.25}$$

Furthermore, thermal stress contribution to total flow stress was considered as a summation of strength due to general obstacles (σ_{gen}) and solid solution (σ_{sol}). The strength contribution from the general obstacles was expressed as,

$$\sigma_{gen} = S_{dis} G_T \left[1 - \left(\frac{k_B T}{A_{dis} G_T b^3} ln\left(\frac{\dot{\varepsilon}_{rf}}{\dot{\varepsilon}}\right)\right)^{1/q}\right]^{1/p}, \tag{1.26}$$

where S_{dis} and A_{dis} are calibration parameters and $\dot{\varepsilon}_{rf}$ is a constant. The exponents $0 < p < 1$ and $1 \leq q \leq 2$ are related to the shape of the energy barrier .The strength contribution form the solute hardening was a function of temperature and the atomic concentration which and expressed as,

$$\sigma_{sol} = \frac{\sigma_{sol}^{ref}}{G} G(T)\left(1 - \left(\frac{T}{T_0^{sol}}\right)^{\frac{2}{3}}\right)^{\frac{3}{2}}, \tag{1.27}$$

Where, σ_{sol}^{ref} the reference value at 0 K and T_0^{sol} was set to 800 K

Model has been simplified to account for dynamic strain aging and incorporated the additional contributions to flow stress from the Hall-Petch effect and solute hardening.

1.3.6. R. Wang et al. Model, 2018

Wang et al. [35] proposed a model to study the hot deformation behavior of 2Cr11Mo1VNbN martensitic stainless steel. WH and DRV was initially considered to estimate the flow response. Afterwards a semi empirical model was utilized to take care of recrystallize part. The evolution of dislocation density was formulated by considering the production and annihilation of dislocations as,

$$\frac{d\rho}{d\varepsilon} = U - \Omega\,\rho \quad , \tag{1.28}$$

Constants have the conventional sense. Strength contribution from dislocations was given as,

$$\sigma_{dis} = \alpha G b\,\sqrt{\rho} \tag{1.29}$$

By invoking the concept of DRX, total strength was further estimated as,

$$\sigma = \sigma_{drv} - (\sigma_{sat} - \sigma_{ss})\left\{1 - exp\left[(-k)\left(\frac{\varepsilon - \varepsilon_c}{\varepsilon_p}\right)^n\right]\right\} \quad , \tag{1.30}$$

where σ_{sat} and σ_{ss} are saturated stress and steady-state stress, respectively. $\varepsilon, \varepsilon_c, \varepsilon_p$ are true strain, critical strain, and peak strain, respectively. k and n are the material constants.

1.3.7. H. Li et al. Model, 2019

Li et al. [36] established a model to simulate microstructure evolution during hot deformation of alloy Ti-5.4Al-3.7Sn-3.3Zr-0.5Mo-0.4Si. The total flow stress was comprised of thermal and athermal stress component.

$$\tau = \underbrace{\tau_{th}}_{thermal} + \underbrace{\tau_{\mu}}_{athermal} \tag{1.31}$$

The thermal component of flow stress was estimated as [32, 37],

$$\tau_{th} = \tau_0 \left[1 - \left(\frac{k_B T}{\Delta f_0 G b^3} \, ln\left(\frac{\dot{\varepsilon}_{ref}}{\dot{\varepsilon}}\right) \right)^{\frac{1}{q}} \right]^{\frac{1}{p}} \tag{1.32}$$

where τ_0 is zero temperature yield stress, Δf_0 is the energy barrier to overcome the dislocation, $\dot{\varepsilon}_{ref}$ is the reference strain rate and the exponents $0 < p < 1$ and $1 \leq q \leq 2$ are related to the shape of the energy barrier.

Furthermore, the athermal stress is expressed [38],

$$\tau_\mu = \alpha G b \sqrt{\rho}_i + K_{HP} l^{-\frac{1}{2}} \quad , \tag{1.33}$$

where *l* is the lamellar thickness. The first term in Equation (1.33) represents strain hardening due to dislocation interaction and the second term is strengthening effect due to grain boundary. Hall-Petch coefficient equation is adopted from the literature [39],

$$K_{HP} = HG\sqrt{b} \ , \tag{1.34}$$

where *H* is factor of Hall-Petch parameter.

The evolution of dislocation density considers the strain hardening and dynamic globularization and expressed as [32, 40],

$$\dot{\rho}_i = \dot{\varepsilon}\left(k_1\sqrt{\rho_i} - k_2\rho_i\right) - \frac{\dot{S}}{(1-S)}\rho_i \varepsilon^{c_2} \tag{1.35}$$

The evolution of dynamic globularization is expressed in the following form.

$$\dot{S} = c_0(1-S)\dot{\varepsilon}^{c_1} M_{gb} P/l \tag{1.36}$$

Where S is the dynamic globularization coefficient, c_0 is the material constant and M_{gb} is the grain boundary mobility and $P = \rho_i G b^2/2$ is pressure on the grain boundary due dislocation accumulation across the grain boundary.

Model [36] predicted the influence of the initial alpha lamellar thickness on the flow stress in addition to temperature and strain rate. The athermal and thermal component of flow stress was also predicted with change in the initial alpha lamellar thickness for the explored conditions.

1.3.8. Surya D. Yadav et al. Model, 2019

Yadav et al. [41] proposed a model to study the deformation behavior of 304HCu austenitic stainless steel. Model relied on the internal variable like forest dislocation density and mobile dislocation density and mean free path. The evolution of forest dislocation density with respect to plastic strain was expressed as [27],

$$\frac{d\rho_f}{d\varepsilon_p} = \left[\frac{M}{b\lambda_{mean}} - MK_2\rho_f\right] \quad (1.37)$$

The other internal variables that are mean free path and mobile dislocation density can be expressed in terms of plastic strain as [27, 42],

$$\frac{d\lambda_{mean}}{d\varepsilon_p} = -K_{L_m}[\lambda_{mean} - \lambda_{ms}] \quad (1.38)$$

$$\frac{d\rho_m}{d\varepsilon_p} = -\left[\frac{M}{b\lambda_{mean}} - \frac{M}{b\lambda_{ms}}\right]. \quad (1.39)$$

Furthermore, the flow stress response was predicted as per the Taylor Hardening approach with considering the forest dislocation density as,

$$\sigma = \sigma_0 + M\alpha G b\sqrt{\rho_f} \quad (1.40)$$

Model predicted the tensile flow curves of 304HCu austenitic stainless steel, focusing on three key internal variables. It was found that forest dislocation density has the major role in influencing the flow stress response.

1.4. Empirical based creep models

1.4.1. M. McLean and B. F. Dyson Model, 2000

McLean and Dyson [43] proposed CDM based model to predict the creep curves of 12% Ctr steel. The creep strain was estimated as per the following equation,

$$\dot{\varepsilon}_{cr} = \dot{\varepsilon}_0 \frac{(1 + D_d)}{(1 - D_s)} \sinh\left[\frac{\sigma(1 - H)}{\sigma_0(1 - D_{ppt})}\right] \tag{1.41}$$

In Equation (1.41) $\dot{\varepsilon}_0$ is a constant, D_d is damage due to dislocation, D_s is damage due to solute depletion and D_{ppt} is damage due to precipitate coarsening, σ is applied stress, H is internal stress and σ_0 is the available stress for dislocation motion, in the absence of any obstacle. Model worked well but relys on the multiple fitting parameter to produce the creep curves for 12% Cr steel. The influence of temperature and stress on the creep curve were also predicted by model.

1.4.2. Y. Yin and R. Faulkner Model, 2006

Yin and Faulkner [44] developed a model by considering the CDM based approach for P92 steel. The creep rate was defined as per Equation (1.42) based on the damage due dislocations, solute depletion, precipitate coarsening and damage due to cavitation.

$$\dot{\varepsilon} = \frac{\dot{\varepsilon}_0}{(1 - D_d)(1 - D_s)} \sinh\left[\frac{\sigma(1 - H)}{\sigma_0(1 - D_{ppt})(1 - D_N)}\right] \tag{1.42}$$

The model included an additional damage parameter D_N, related to creep void formationand it was able to produce the creep curves up to tertiary regime for P92 steel.

1.4.3. N. Bonora and L. Esposito Model, 2008

A unified creep model for pure aluminum was developed by Bonora et al. [45], which considered dislocation climb mechanism coupled with CDM approach. The creep strain was estimated according to following equation,

$$\dot{\varepsilon} = \frac{kD_v}{b^2}\left(\frac{\sigma}{\sigma_0(1-D)}\right)^n, \tag{1.43}$$

In Equation (1.43) k is material dependent constant, D is damage parameter and n is the stress exponent. Damage parameter is associated with irreversible thermodynamics based approach and estimated as per the following equation,

$$D = \dot{\lambda}\frac{\partial f_D}{\partial Y}, \tag{1.44}$$

where $\dot{\lambda}$ is plastic multiplier, f_d is damage dissipation potential and Y is damage variable. Model worked well for the large portion of tertiary creep regime.

1.4.4. B. Xiao et al. Model, 2019

Xiao et.al [46] proposed the deformation-mechanism-based creep model for G115 steel. The creep strain was estimated as per the Equation (1.45) by considering the GBS (grain boundary sliding), IDG (intragranular deformation glide) and IDC (intragranular deformation climb) as,

$$\dot{\varepsilon} = \dot{\varepsilon}_{GBS} + \dot{\varepsilon}_{IDG} + \dot{\varepsilon}_{IDC}\ , \tag{1.45}$$

where $\dot{\varepsilon}_{GBS}$, $\dot{\varepsilon}_{IDG}$, and $\dot{\varepsilon}_{IDC}$ are the minimum creep rates due to GBS, IDG, and IDC, respectively and estimated as per the following equations,

$$\dot{\varepsilon}_{GBS} = A_1\exp\left[-\frac{Q_1}{RT}\right]\sigma^p \tag{1.46}$$

$$\dot{\varepsilon}_{IDG} = A_2\exp\left[-\frac{Q_2}{RT}\right]\sigma^n \tag{1.47}$$

$$\dot{\varepsilon}_{IDC} = A_3 \exp\left[-\frac{Q_3}{RT}\right] \sigma^m \qquad (1.48)$$

Where *p*, *n* and *m* are the stress exponents for GBS, IDG and IDC, respectively. Model worked well for complete creep regime.

1.5. Physics-based creep models

Unlike the empirical-based creep models, which only simulates the creep curves, the physics-based creep model provides insights about the microstructure evolution. In past several creep models were developed and discussed in next subsections.

1.5.1. N. M. Ghoniem et al. Model, 1990

Ghoniem et al. [47] proposed a creep model for HT-9 martensitic stainless steel. It was based on three different dislocations configurations namely, mobile, static (ρ_s) and boundary (ρ_b) and the creep strain was estimated from fundamental Orowan equation as [48],

$$\dot{\varepsilon} = b\rho_m v_{gl} \qquad (1.49)$$

The model predicted the primary and secondary creep regimes, though the substructure evolution was not studied by the model.

1.5.2. H. Magnusson et al. Model, 2007

Magnusson et al. [49] proposed a creep model for a 9% Cr steel using two different dislocation configurations (free and immobile) and subgrain size. The evolution of the immobile dislocation density within subgrains was expressd as,

$$\frac{d\rho_i}{dt} = \frac{\dot{\varepsilon}M}{b} 4d_{lock} \frac{(n_{slip}-1)}{n_{slip}} \rho_{free} - 2M_{cl}T_L\rho_i^2 \quad , \qquad (1.50)$$

where d_{lock} is the critical distance for the formation of dislocation lock, n_{slip} is number of slip systems, M_{cl} is dislocation climb mobility and T_L is dislocation line tension. Similarly, the evolution of free dislocation density was expressed as,

$$\frac{d\rho_{free}}{dt} = \frac{1}{\lambda_{mean}} \frac{\dot{\varepsilon}M}{b} - 2\rho_{free}\frac{\dot{\varepsilon}M}{b}\left[\frac{d_{dip}}{n_{slip}} + \frac{2d_{lock}(n_{slip}-1)}{n_{slip}}\right] \tag{1.51}$$

where d_{dip} is dipole capture spacing.

The estimation of creep rate was based on Norton's equation and back stress stress concept and estimated as,

$$\dot{\varepsilon}_{disl} = A_N e^{-\frac{Q_C}{RT}}\left(\sigma_{app} - \sigma_{back,tot}\right)^N, \tag{1.52}$$

where A_N is constant, Q_C is activation energy for creep, σ_{app} is applied stress, $\sigma_{back,tot}$ is total back stress contribution form work hardening and particle strengthening and N is creep exponent. Back stress in either subgrain interior or subgrain boundaries was summarised as,

$$\sigma_{back,i} = \alpha MGb\sqrt{\rho_i} + \frac{2MT_L}{bL_{i,tot}}, \tag{1.53}$$

Herein, $L_{i,tot}$ is the total interparticle spacing. Subgrain growth takes place by glide and climb of dislocations and was related to the dislocation climb mobility as [50],

$$\frac{dR_{sub}}{dt} = 3\frac{M_{cl}T_L}{2R_{sub}}\left[1-\left(\frac{R_{sub}}{R_{sub,inf}}\right)^2\right]^2 \quad , \tag{1.54}$$

where $R_{sub,inf}$ is the limiting subgrain size. Model [49] was based on heterogeneous dislocation structure observed in 9 to 12 pct Cr steels and dislocation density evolution was modeled along with creep curves.

1.5.3. H. Semba et al. Model, 2008

Semba et al. [51] proposed a model for 9 % Cr steel that considered the constitutive equations adapted from by Kadoya et al. [52],

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \frac{1 + D_d}{1 - \left(1 - \frac{c_e}{c_0}\right) D_s} \sinh\left[\frac{\sigma(1 - H)}{\sigma_0\left(1 - D_{ppt}\right)}\right], \tag{1.55}$$

where D_d is damage is due to dislocation accumulation, c_e is solute concentration at equilibrium, c_0 is the initial solute concentration. Model predicted the creep curves and temperature and stress influence was addressed. It incorporated the subgrain formation and MX carbonitride precipitate coarsening identified as one of the primary causes of tertiary creep.

1.5.4. B.F. Dyson Model, 2008

Dyson et al. [53] proposed a model to produce the minimum creep rate for Nimonic 90. The dispersion-controlled shear creep rate was expressed as,

$$\frac{d\gamma}{dt} = 1.6\varphi_p \rho \left(\left(\frac{\pi}{4\varphi_p}\right)^{1/2} - 1\right) C_j D v \ \ \sinh\left(\frac{\tau_D b^2 \lambda_p}{k_B T}\right) \quad , \tag{1.56}$$

where φ_p is volume fraction of hard particle, c_j is the dislocation jog density, and D_v is volume diffusion coefficient, τ_D is effective shear stress and λ_p is interparticle spacing. Observed minimum creep rate was closely aligned with the model predictions, indicating reasonable agreement. Model suggested that minimum creep rate was notably affected by the precipitate spacing.

1.5.5. F. Krumphal et al. Model, 2009

Krumphal et al.[54] proposed a creep model for hot work tool steel. It was based on three different dislocations configurations namely, mobile, static and boundary and the creep strain was estimated from fundamental Orowan equation as [48],

$$\dot{\varepsilon} = b\rho_m v_{gl} \tag{1.57}$$

The predicted creep strain was compared with output of FEM simulation and experimental data, though the substructure evolution was not studied by the model.

1.5.6. M. Basirat et al. Model, 2012

Basirat et al. [55] proposed a hybrid model (combination of physics based approach and CDM) to study the creep deformation behavior of a 9Cr-1Mo steel. The important internal variables in this model were ρ_m and ρ_{dip}. Coupling it with CDM approach, damage due to precipitates coarsening, solute depletion and cavitation were included to model the complete creep curves The creep strain was estimated by Equation (1.58) modified Orowan equation [48].

$$\dot{\varepsilon} = \frac{b\rho_m v_{gl}}{M(1-D_S)(1-D_{ppt})(1-D_{cav})} \tag{1.58}$$

Where D_{cav} is the damage due to cavitation.

The evolution of mobile dislocation and dipole dislocation density was expressed as,

$$\dot{\rho_m} = \frac{M\dot{\varepsilon}}{b\lambda_{mean}} - \frac{4M\dot{\varepsilon}d_{dip}\rho_m}{bn_g} - \frac{2M\dot{\varepsilon}d_{dip}}{b}, \tag{1.59}$$

$$\dot{\rho_{dip}} = \frac{2M\dot{\varepsilon}d_{dip}}{b} - \frac{2M\dot{\varepsilon}d_{spon}\rho_{dip}}{bn_g} - \rho_{dip}\frac{4v_{cl}}{d_{dip}-d_{spon}} \tag{1.60}$$

where n_g is the number of active slip planes.

Modeled [55] creep curves showed a reasonable agreement with experimental creep curves up to large portion of tertiary creep regime, though internal variables were not discussed thoroughly.

1.5.7. Y.K. Kim et al. Model, 2016

Kim et al. [56] proposed a model to study the creep deformation behavior of a nickel based super alloy. Model accounted for dislocation creep and grain boundary sliding for the calculation of the minimum creep strain rate as,

$$\dot{\varepsilon}_m = A_1\varphi(1-\varphi)\left(\frac{1}{\varphi^{\frac{1}{3}}}-1\right),\frac{D_L G b}{k_B T}\ (\lambda\gamma')^2\left(\frac{\Gamma}{Gb}\right)^3\left(\frac{(\sigma-\sigma_{app})}{G}\right)^5 + A_2\frac{D_L G b}{k_B T}\ \left(\frac{b}{g}\right)^2\left(\frac{\sigma}{G}\right)^2 \quad (1.61)$$

Where A_1 and A_2 are adjustable model parameters, φ is volume fraction of γ' precipitates and Γ is stacking fault energy. Furthermore, the tertiary creep regime was modelled with the following empirical relation,

$$\dot{\varepsilon}_t = \dot{\varepsilon}_m(1+C\varepsilon), \quad (1.62)$$

where C is a constant related to damage. Total creep strain rate was considered to be a summation of minimum creep rate and tertiary creep rate as,

$$\dot{\varepsilon}_{total} = \dot{\varepsilon}_m + \dot{\varepsilon}_t \quad (1.63)$$

Model demonstrated the ability to replicate the complete creep curves of numerous nickel-based superalloys with a reasonable level of agreement. The influence of the stacking fault energy was also addressed by the model, in addition to effect of temperature and stress on creep curves.

1.5.8. Surya D. Yadav et al. Model, 2016, 2018

Yadav et.al. [57, 58] developed the hybrid model by combining physically based model with CDM based approach. The creep strain rate was defined in the following form,

$$\dot{\varepsilon} = f\left(\rho_m, \rho_b, \rho_{dip}, R_{sub}, T, \sigma, N_v, r_{p,i}, D_{cav}, D_{ppt}\right), \quad (1.64)$$

where N_v is number density of precipitates, $r_{p,i}$ is the radius of $M_{23}C_6$ carbide and MX carbonitride types of the precipitate, where M=Fe, Cr and X=C, N, D_{ppt} is the related to coarsening of $M_{23}C_6$ carbides and MX carbonitrides precipitates and D_{cav} is damage due to cavitation. Rate of softening due to coarsening of precipitates was expressed as,

$$\dot{D}_{(ppt),l} = \frac{k_p}{(l-1)}\left(1 - \dot{D}_{(ppt),l}\right)^l, \quad (1.65)$$

where K_p is a constant related to the Ostwald ripening and $l=4$ and 6 $M_{23}C_6$ carbides and MX carbonitrides precipitates, respectively. Similarly, the damage rate due to cavitation was expressed as,

$$\dot{D}_{cav} = (A.\varepsilon.\dot{\varepsilon}), \quad (1.66)$$

where A is an adjustable parameter. Creep strain rate was estimated by the modification of Orowan equation including the softening due to cavitation and coarsening of precipitates as,

$$\frac{d\varepsilon}{dt} = \frac{b\rho_m v_{gl}}{M(1 - D_{ppt})(1 - D_{cav})}, \quad (1.67)$$

Model simulated the creep curves for up to a large portion of the tertiary creep regime for P91 and P92 steels. The influence of temperature and stress on the creep curve was also predicted by the model. In addition to this, it discusses the microstructure-based variables with ongoing creep to provide more insights into the evolved microstructure.

1.5.9. C.Ó Murchú et al. Model, 2017

Murchu et al. [59] proposed a CDM based model to address the deformation behavior in P91 steel that was adopted from the research work of Hayhurst and co-workers [60, 61]. The creep strain was estimated as per the following expression,

$$\dot{\varepsilon}_{cr} = \dot{\varepsilon}_0 exp\left(-\frac{\Delta f}{k_B T}\right) \sinh\left[\frac{\sigma(1-H)}{\sigma_0\left(1-D_{ppt}\right)(1-D_{cr})}\right] \tag{1.68}$$

where Δf is Helmholtz free energy, D_{cr} is damage due to chromium depletion. Model predicted the complete creep curves including the temperature and stress influence. Additionally, the model was also capable of addressing the detrimental effect of Al content on the creep rupture behaviour of P91 steel.

1.5.10. S. Wu et al. Model, 2022

A microstructure-based creep model was developed by Wu et al. [62] to predict the creep curves for additively manufactured nickel-based superalloy. Total creep strain rate was considered to be a summation of dislocation creep and grain boundary sliding and expressed as,

$$\frac{d\varepsilon}{dt} = \frac{d\varepsilon_{dislocation}}{dt} + \frac{d\varepsilon_{GBS}}{dt} \tag{1.69}$$

Creep strain rate due to movement of dislocations was estimated with the following expression,

$$\frac{d\varepsilon_{dislocation}}{dt} = \frac{\rho_m}{Mh}\varphi\lambda_{mean}C_j D_L \sinh\left(\frac{\sigma b^2 \lambda_{mean}}{M k_B T}\right) \tag{1.70}$$

where h is dislocation climb distance against precipitates.

Based on the grain boundary sliding mechanisms, creep strain rate was estimated with the following expression as,

$$\frac{d\varepsilon_{GBS}}{dt} = \frac{AD_{gb}Gb}{k_BT}\left(\frac{b}{g}\right)^q \left(\frac{(r_{gb}+\lambda_{gb})}{b}\right)^{q-1} \left(\frac{\left(\frac{\sigma}{M}-\tau_g\right)\left(\frac{\sigma}{M}-\tau_c\right)}{G^2}\right), \quad (1.71)$$

where A is the material constant, the exponent q having a value of 1, 2, 3 for the conditions of no grain boundary particles, discrete particles and continuous particles, whereas τ_g and τ_c represents the glide and climb resistance for the grain boundary sliding.

Model predicted the large portion of the creep curves. Effect of anisotropy on creep due to the additive manufacturing was also well elucidated by the model. Moreover, to achieve a longer creep life, the model indicated that homogenization heat treatment as a critical factor.

1.6. Problem definition

It can be said that, several flow stress models [23-25] were developed over the past decades to simulate the flow curves, primarily based on simple empirical descriptions . This type of empirical models [23-25] uses many constants that are without any physical meaning. On the other hand, Mean-field physical modeling of flow stress offers a mathematical framework to understand the deformation behavior of alloys and to link their microstructure with flow properties. Significant advancement has been done in this field [4, 5, 26, 29, 30, 34-37, 41, 63-65] but some open problems still exists with these models. Following issues were observed with respect to flow stress models,

- Most of the flow stress models predicts the microstructure evolution along with flow stress response but the velocity of dislocations and influence on recrystallization phenomena was not discussed.
- All the experimental curves are fitted with the models, limiting the prediction capabilities.

- A physical based model that incorporates annealing twin density effect and explains the microstructural evolution during each time step of plastic deformation for low stacking fault energy material was not reported.
- Individual contribution of different type of strengthening was rarely addressed.

Similarly, a good advancement was achieved in the creep modelling field following an approach in which creep rate is modelled as,

$$\dot{\varepsilon} = f\left(\rho_m, \rho_b, \rho_{dip}, R_{sub}, T, \sigma_{appl}, N_v, r_p, D_{cav}, D_{ppt}\right), \tag{1.72}$$

The problem lies in such a way that if models address complete creep curve then microstructural evolution and all other important parameters were not demonstrated [14, 20, 43-46, 51, 53, 56, 59, 66]. Impact of all internal variables during the creep exposure is very important following issues were observed with existing creep models:

- Complex dislocation climb velocity models were used and temperature dependent shear modulus was not incorporated.
- Evolution of some variables that were ignored in the literature, those are boundary dislocation spacing, subgrain boundary mobility, dipole capture spacing, climb stress, mean radius of precipitates.
- Evolution of damage due to two different types of precipitates was not demonstrated separately. Temperature and time dependent mobility model for subgrain boundary migration was not implemented.
- Slip systems were not incorporated in rate equations of microstructural evolution and influence of stacking fault energy on dislocation velocities was not considered.

In light of these issues, physics based creep and flow stress models were developed in the subsequent chapters to address these issues. In each of the chapter, an improved model is presented that fills the gap in the literature to some extent.

Chapter 2 addresses the problems 1 to 2, while Chapter 3 is focused on problem number 3 to 4. Chapter 4 addresses the problems 5 to 7, Chapter 5 is focused on problem 8 and Chapter 6 deals with problems 5, 7.