

FATIGUE DESIGN 2021, 9th Edition of the International Conference on Fatigue Design

## Estimating the fatigue thresholds of additively manufactured metallic materials with consideration of defects

D. Rigon and G. Meneghetti\*

*University of Padova, Department of Industrial Engineering, via Venezia 1 – 35131 Padova, Italy*

---

### Abstract

The fatigue limits of defective alloys can be estimated by using classical models which require the experimental evaluation of some material properties. In the case of the Atzori-Lazzarin-Meneghetti model (ALM), the experimental fatigue limit of the “defect-free” material,  $\Delta\sigma_0$ , and the threshold stress intensity factor for long cracks,  $\Delta K_{th,LC}$ , are required to evaluate the transition of the Kitagawa-Takahashi diagram, i.e. the fatigue limits of small defects. Recently, by using data taken from the literature an empirical model has been calibrated for evaluating  $\Delta K_{th,LC}$  of several wrought as well as additively manufactured (AM) alloys for different load ratios (-1, 0 and 0.5), where the sole parameters required are the hardness (HV) and a properly defined microstructural lengths,  $l$ . As to the “defect-free” plain material fatigue limit, i.e.,  $\Delta\sigma_{0(R)}$ , for different load ratios, the fatigue limit estimation for  $R = -1$  ( $\Delta\sigma_{0(R=-1)} = f(HV)$ ) has been corrected by using a classical mean-stress-based model. As a result, the ALM model was defined and compared with short cracks/small defects fatigue tests results taken from the literature. A good correlation has been found between theoretical estimation and experimental results obtained from the fatigue tests on defective AM alloys with  $R = -1$  and 0.1.

© 2021 The Authors. Published by Elsevier B.V.

This is an open access article under the CC BY-NC-ND license (<https://creativecommons.org/licenses/by-nc-nd/4.0>)

Peer-review under responsibility of the scientific committee of the Fatigue Design 2021 Organizers

*Keywords:* Fatigue limit; Near-Threshold; Additive Manufacturing; Material length parameters; Hardness; Defects

---

---

\* Corresponding author. Tel.: +39-049-8276751; fax: +39-049-8276785

*E-mail address:* [giovanni.meneghetti@unipd.it](mailto:giovanni.meneghetti@unipd.it)

## Nomenclature

$a_{0,est(R)}$	estimated El-Haddad-Smith-Topper material length parameter for a given R
$a_{eff}$	effective defect size ( $a_{eff}=\alpha^2\cdot\sqrt{area}$ or $a_{eff}=\alpha^2\cdot a$ )
$l$	microstructural length parameter
R	load ratio ( $R=\sigma_{min}/\sigma_{max}$ )
$\alpha$	shape factor to evaluate the Mode I stress intensity factor (SIF)
$\Delta\sigma_{0,(R)}$	defect-free fatigue limit in terms of nominal stress range (maximum value minus minimum value) for a give load ratio
$\Delta\sigma_g$	range (maximum value minus minimum value) of the nominal stress referred to the gross area
$\Delta\sigma_{g,th,(R)}$	threshold range of the nominal stress referred to the gross area for a given R
$\Delta K_{th,LC,est,(R)}$	estimated threshold SIF range of long cracks for a given load ratio R
$\Delta K_{th,SC}$	threshold SIF range of mechanically short cracks/small defects
$\sqrt{area}$	square root of the area of a defect projected onto the plane perpendicular to the maximum principal stress
ALM	Atzori Lazzarin Meneghetti model
AM	Additively Manufacturing
CM	Conventionally Manufactured materials
EST	El Haddad Smith Topper model
LOF	Lack of Fusion defect
LEFM	Linear Elastic Fracture Mechanics

## 1. Introduction

The fatigue design of Additively Manufactured (AM) alloys is one of the main challenges that need to be addressed in several industrial sectors (aerospace, aeronautic and automotive) that take advantage of complex high-performance lightweight components. It is known that the combination of process-inherent microstructural features, residual stresses, surface roughness and distribution of defects implies a different fatigue behaviour in metal materials processed by conventional (CM) as well as additive manufacturing (AM) technologies (Xu et al. 2015; Carlton et al. 2016; Li et al. 2016; Wang et al. 2016; Lewandowski and Seifi 2016; Meneghetti et al. 2017; Rigon et al. 2018; Morettini et al. 2019; Mooney et al. 2019; Chern et al. 2019; Afkhami et al. 2019; Solberg and Berto 2019; Carneiro et al. 2019; Gockel et al. 2019; Damon et al. 2019; Kan et al. 2019; Razavi et al. 2020). In particular, the distribution of defects and its interaction with the microstructure play a fundamental role in the assessment of the fatigue behaviors of AM alloy (Zerbst et al. 2021; Murakami et al. 2021). Classical approaches such as the El Haddad Smith Topper model (El Haddad et al. 1979a, b) or its extension proposed by Atzori Lazzarin Meneghetti (Atzori et al. 2003, 2005) can be useful for estimating the fatigue thresholds of alloys containing short cracks, defects, long cracks as proposed recently (Beretta and Romano 2017; Hu et al. 2020; Rigon and Meneghetti 2020). Both models require two material properties, namely the defect-free fatigue limit  $\Delta\sigma_{0,(R)}$  and the threshold stress intensity factor for long cracks  $\Delta K_{th,LC,(R)}$  for a given load ratio (R). However, these material properties are often unavailable in the design phase of a component and their determination needs time-consuming experimental tests. To address this problem, Rigon and Meneghetti have recently proposed an empirical equation for evaluating  $\Delta K_{th,LC,(R)}$  for  $R = -1$ ,  $R = 0$  and  $R = 0.5$  that requires only the Vickers Hardness (HV) and a material-dependent microstructural length ( $l$ ) (Rigon and Meneghetti 2020) (Rigon and Meneghetti 2021). To rationalize the effect of the load ratio, the models based on  $\Delta K$  and  $K_{max}$  can be used (Sadananda et al. 2019; Bang and Ince 2020). As to the defect-free material fatigue limit required for the EST and ALM models, i.e.  $\Delta\sigma_{0,(R)}$  for different load ratios, the fatigue limit for  $R = -1$  estimated by means of HV has been corrected by using a classical mean stress-based model as a function of R and HV only. The aim of the present paper is to summarize the comparison between experimental results taken from the literature and theoretical estimations of the fatigue thresholds of AM materials for  $R = -1$  and  $R = 0.1$ .

## 2. Theoretical background

The empirical equation for the estimation of  $\Delta K_{th,LC,(R)}$  was calibrated for a certain list of materials in (Rigon and Meneghetti 2020) and (Rigon and Meneghetti 2021), to which the reader is referred, and it is the following:

$$\Delta K_{th,LC,(R)} = \alpha_R \cdot l^{\beta_R + \gamma_R} \cdot HV^{\delta_R} \quad (1)$$

where  $\alpha_R$ ,  $\beta_R$ ,  $\gamma_R$ ,  $\delta_R$  are coefficients that depend on the load ratio R. The  $l$  parameter is a microstructure-dependent length that is measurable by following definitions proposed by (Yoder et al. 1983)(Rigon and Meneghetti 2020, 2021). The coefficients of Eq. 1 have been calibrated for R equal to -1, 0, and 0.5 and the resulting values are listed in Table 1. In Eq. (2) the units of the parameters  $\Delta K_{th,LC,(R)}$ ,  $l$  and HV are [ $MPa\sqrt{m}$ ], [ $\mu m$ ] and [ $kgf/mm^2$ ], respectively.

Table 1. Calibrated coefficients of Eq. (1) for different load ratios R.

R	$\alpha_R$	$\beta_R$	$\gamma_R$	$\delta_R$
-1	4.5	0.127	229	-0.81
0	1.82	0.165	53.52	-0.53
0.5	1.68	0.203	5.94	-0.26

Eq. (1) with coefficients reported in Table 1 proved to estimate  $\Delta K_{th,LC,(R)}$  within an error band of  $\pm 20\%$ .

Regarding the defect-free material, the fatigue limit of for R = -1 can be estimated from the HV by using the following equation (Murakami 2019):

$$\frac{\Delta\sigma_{0,est,(R-1)}}{2} = 1.6 \cdot HV \quad (2)$$

It is well known that Eq. (2) is valid for steels and some nonferrous metals having HV lower than 400. However, in this theoretical framework,  $\Delta\sigma_{0,est,(R-1)}$  has been evaluated by Eq. (2) also for materials having HV > 400 by considering it as a “virtual” defect-free fatigue limit.

Combining the Goodman Smith model with Eq. (2), the effect of the mean stress on the fatigue limit can be evaluated by means of the following equation as proposed in (Rigon and Meneghetti 2021):

$$\frac{\Delta\sigma_{0,est,(R)}}{2} = 3.2 \cdot HV \frac{(1-R)}{(3-R)} \quad (3)$$

By using Eqs. (1) and (3) for a given load ratio, it is possible to draw the ALM model to estimate the fatigue limit of defective materials, i.e. the fatigue thresholds (Atzori et al. (2003), Atzori et al. (2005)):

$$\Delta\sigma_{g,th,(R)} = \Delta\sigma_{0,est,(R)} \sqrt{\frac{a_0}{a_0 + a_{eff}}} \quad (4)$$

where  $a_{eff}$  and  $a_0$  are defined as follows:

$$a_{eff} = \alpha^2 \sqrt{area} \quad (5)$$

$$a_0 = \frac{1}{\pi} \left( \frac{\Delta K_{th,LC,(R)}}{\Delta\sigma_{0,est,(R)}} \right)^2 \quad (6)$$

Eq. (5) holds for internal and surface defects where the shape factor  $\alpha$  is equal to 0.5 and 0.65, respectively (Murakami 2019). It can be noted that Eq. (6), written in this form, is a material property because  $\alpha$  have been included in Eq. (5) (Atzori et al. 2003).

Finally, combining Eq (1), (3) and (6) the ALM model can be estimated for a given load ratio by using only HV and  $l$ .

### 3. Literature data

The material fatigue properties  $\Delta\sigma_{0,est(R)}$  (Eq. 3),  $\Delta K_{th,LC,est(R)}$  (Eq. 1) and  $a_{0,est(R)}$  (Eq. 6) of AM alloys for  $R=-1$  and  $R\cong 0$  are summarised in Table 2 (Wycisk et al. 2014; Masuo et al. 2018; Hu et al. 2020; Romano et al. 2020; Qian et al. 2020; Pellizzari et al. 2020; Rigon and Meneghetti 2020; Liu et al. 2020; Andreau et al. 2021).

All refs. summarised in Table 2 report constant amplitude fatigue test results where the size of the killer defect was evaluated after failure. The reader is referred to (Rigon and Meneghetti (2020) (2021)) for details regarding the additive manufacturing process, the fatigue testing conditions and the definition of the microstructural size  $l$ .

Table 2. Material properties of AM materials taken from the literature and estimated with Eq. (1), (3) and (6) for  $R = -1$  and  $R \cong 0$  (Rigon and Meneghetti (2020) (2021)).

Ref.	Material	$\sigma_{UTS}$ [MPa]	$\sigma_Y$ [MPa]	R	definition of $l$	$l$ [ $\mu\text{m}$ ]	HV [kg/mm <sup>2</sup> ]	$\Delta K_{th,LC,est}^\circ$ [MPa $\sqrt{\text{m}}$ ]	$\Delta\sigma_{0,est}^\wedge$ [MPa]	$a_{0,est}^+$ [ $\mu\text{m}$ ]
(Masuo et al. 2018)	Ti6Al4V (EBM)	1046	/	-1	width of $\alpha$ lamellae	$\approx 2$	369	6.82	1181	10.6
	Ti6Al4V (DMLS)	1176	/		width of $\alpha$ lamellae	$\approx 2$	378	6.79	1210	10.0
(Liu et al. 2020)	Ti6Al4V	1079	887		martensite lath width	1	380	6.36	1216	8.71
(Qian et al. 2020)	Ti6Al4V	/	/		width of $\alpha$ lamellae	1.2	380	6.47	1216	9.01
(Romano et al. 2020)	17-4PH				sub-grain cell size/martensite lath width	$\approx 1$	350	6.49	1120	10.7
(Pellizzari et al. 2020)	H13 tool steel	/	/		sub-grain cell size/martensite lath width	0.86	488	5.94	1562	4.60
Rigon and Meneghetti (2020)	MS 300 NT a)	/	/		sub-grain cell size/martensite lath width	0.70	358	6.26	1146	9.50
	MS 300 T a)	/	/		sub-grain cell size/martensite lath width	0.72	555	5.69	1776	3.27
	MS 300 T b)	/	/		sub-grain cell size/martensite lath width	0.9	618	5.70	1978	2.64
(Wycisk et al. 2014)	Ti6Al4V	/	/	0.1	width of $\alpha$ lamellae	0.5	380	3.92	1216	3.31
(Hu et al. 2020)	Ti6Al4V	1267	1094		width of $\alpha$ lamellae	1.5	375	4.26	1200	4.01
(Andreau et al. 2021)	AISI 316L	583	488		sub-grain cell size/martensite lath width	0.5	243	4.53	778	10.8

$^\wedge$  estimated with Eq. (3)

$^\circ$  estimated with of Eq. (1)

$^+$  estimated with Eq. (6)

### 4. Comparison between ALM model and experimental results

The ALM model (Eq (4)) applied to each dataset reported in Table 2 has been reported in Fig. 1 in a log-log diagram where the fatigue threshold  $\Delta\sigma_{g,th(R)}$  and the effective defect size  $a_{eff}$  have been normalized. Therefore, all datasets of Table 2 have been summarized in a single diagram. Fig. 1a reports experimental results relevant to fully reversed fatigue tests, while Fig. 1b is relevant to  $R = 0.1$ . If correlation between the ALM model and experimental results were perfect, the model should separate sharply the results of broken and unbroken specimens, respectively. The resulting correlation is good both for  $R=-1$  and for  $R=0.1$ .

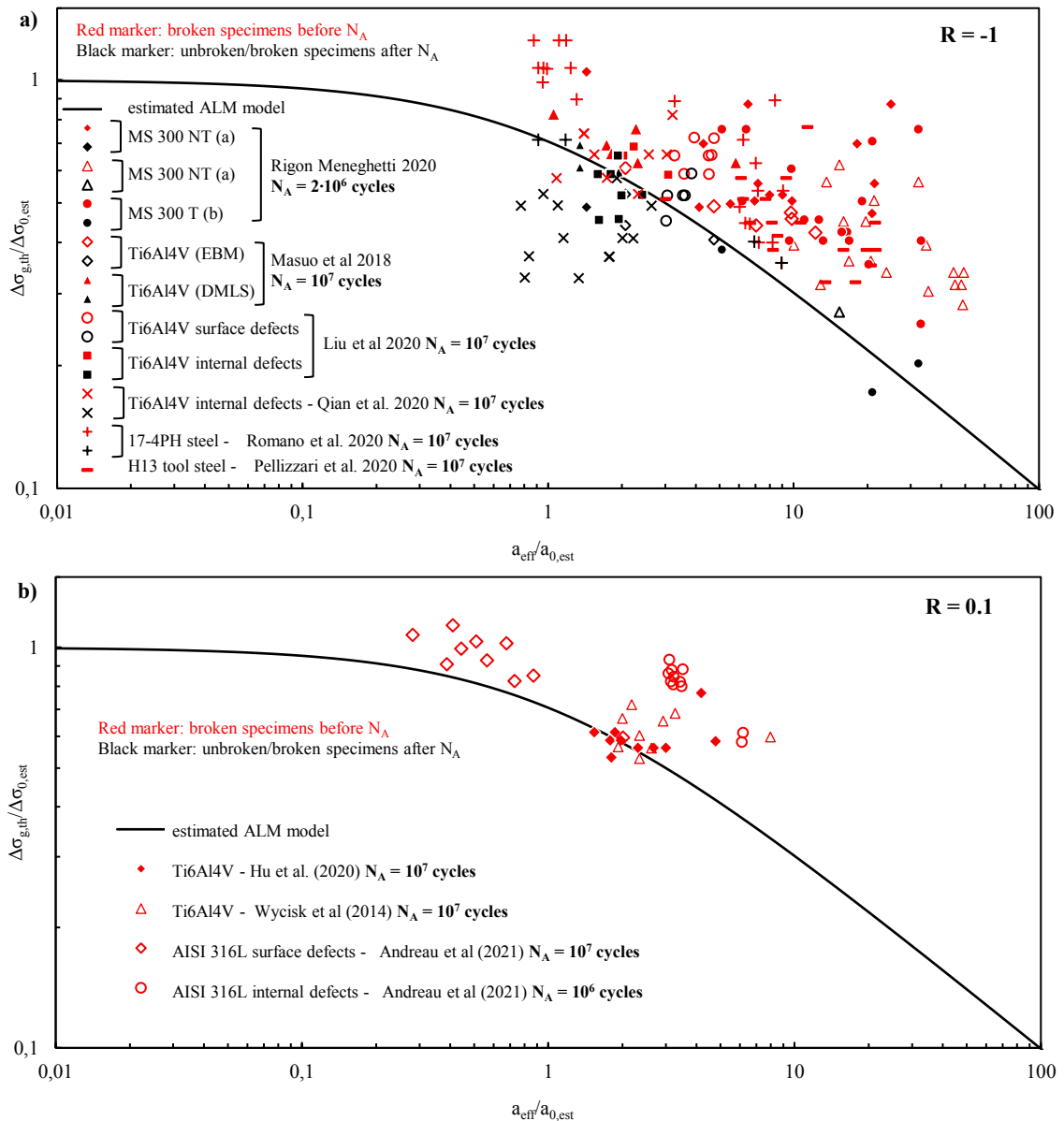


Fig. 1. Comparison between the experimental fatigue test results taken from dataset of Table 2 and fatigue thresholds according to the ALM model (Eq. 4) for (a)  $R=-1$  and (b)  $R=0.1$ .

Interestingly, data relevant to AM 316L steel (Andreau et al. 2021) resulted in good agreement with the theoretical predictions in case of failure relevant to the surfaces defects, whereas estimations relevant to the large artificial internal defects are highly conservative. It is interesting to note that the authors of the original paper (Andreau et al. 2021) underline that the different fatigue behaviour of internal as opposed to surface defects can be explained by the different gaseous environment to which they are exposed.

## 5. Conclusions

A summary of datasets taken from the literature and analysed in previous work by the authors has been presented to highlight the estimation of the fatigue threshold of defective AM alloys by simply measuring the Vickers hardness, HV, and a material-dependent microstructural length  $l$ . Previously, an empirical model based on HV and  $l$  measurements was calibrated for the estimation of the threshold stress intensity factor for long cracks of wrought as well as AM alloys. Combined with the estimation of the defect-free material as a function of HV, the Atzori Lazzarin Meneghetti (ALM) model could be evaluated, and theoretical estimations were compared with a large dataset of fatigue test results obtained on AM metals for load ratios equal to -1 and 0.1. The ALM model exhibited good agreement with the experimental results.

## References

- Afkhami S, Dabiri M, Alavi SH, et al (2019) Fatigue characteristics of steels manufactured by selective laser melting. *Int J Fatigue* 122:72–83. <https://doi.org/10.1016/j.ijfatigue.2018.12.029>
- Andreau O, Pessard E, Koutiri I, et al (2021) Influence of the position and size of various deterministic defects on the high cycle fatigue resistance of a 316L steel manufactured by laser powder bed fusion. *Int J Fatigue* 143:105930. <https://doi.org/10.1016/j.ijfatigue.2020.105930>
- Atzori B, Lazzarin P, Meneghetti G (2003) Fracture mechanics and notch sensitivity. *Fatigue Fract Eng Mater Struct* 26:257–267. <https://doi.org/10.1046/j.1460-2695.2003.00633.x>
- Atzori B, Lazzarin P, Meneghetti G (2005) A unified treatment of the mode I fatigue limit of components containing notches or defects. *Int J Fract* 133:61–87. <https://doi.org/10.1007/s10704-005-2183-0>
- Bang DJ, Ince A (2020) A short and long crack growth model based on 2-parameter driving force and crack growth thresholds. *Int J Fatigue* 141:105870. <https://doi.org/10.1016/J.IJFATIGUE.2020.105870>
- Beretta S, Romano S (2017) A comparison of fatigue strength sensitivity to defects for materials manufactured by AM or traditional processes. *Int J Fatigue* 94:178–191. <https://doi.org/10.1016/j.ijfatigue.2016.06.020>
- Carlton HD, Haboub A, Gallegos GF, et al (2016) Damage evolution and failure mechanisms in additively manufactured stainless steel. *Mater Sci Eng A* 651:406–414. <https://doi.org/10.1016/j.msea.2015.10.073>
- Carneiro L, Jalalahmadi B, Ashtekar A, Jiang Y (2019) Cyclic deformation and fatigue behavior of additively manufactured 17–4 PH stainless steel. *Int J Fatigue* 123:22–30. <https://doi.org/10.1016/j.ijfatigue.2019.02.006>
- Chern AH, Nandwana P, Yuan T, et al (2019) A review on the fatigue behavior of Ti-6Al-4V fabricated by electron beam melting additive manufacturing. *Int J Fatigue* 119:173–184. <https://doi.org/10.1016/j.ijfatigue.2018.09.022>
- Damon J, Hanemann T, Dietrich S, et al (2019) Orientation dependent fatigue performance and mechanisms of selective laser melted maraging steel X3NiCoMoTi18-9-5. *Int J Fatigue* 127:395–402. <https://doi.org/10.1016/j.ijfatigue.2019.06.025>
- El Haddad MH, Smith KN, Topper TH (1979a) Fatigue Crack Propagation of Short Cracks. *J Eng Mater Technol* 101:42. <https://doi.org/10.1115/1.3443647>
- El Haddad MH, Topper TH, Smith KN (1979b) Prediction of non propagating cracks. *Eng Fract Mech* 11:573–584. [https://doi.org/10.1016/0013-7944\(79\)90081-X](https://doi.org/10.1016/0013-7944(79)90081-X)
- Gockel J, Sheridan L, Koerper B, Whip B (2019) The influence of additive manufacturing processing parameters on surface roughness and fatigue life. *Int J Fatigue* 124:380–388. <https://doi.org/10.1016/j.ijfatigue.2019.03.025>
- Hu YN, Wu SC, Wu ZK, et al (2020) A new approach to correlate the defect population with the fatigue life of selective laser melted Ti-6Al-4V. *Int J Fatigue* 105584. <https://doi.org/10.1016/j.ijfatigue.2020.105584>
- Kan WH, Nadot Y, Foley M, et al (2019) Factors that affect the properties of additively-manufactured AlSi10Mg: Porosity versus microstructure. *Addit Manuf* 29:100805. <https://doi.org/10.1016/j.addma.2019.100805>
- Lewandowski JJ, Seifi M (2016) Metal Additive Manufacturing: A Review of Mechanical Properties. *Annu Rev Mater Res* 46:151–186. <https://doi.org/10.1146/annurev-matsci-070115-032024>
- Li P, Warner DH, Fatemi A, Phan N (2016) Critical assessment of the fatigue performance of additively manufactured Ti-6Al-4V and perspective for future research. *Int J Fatigue* 85:130–143. <https://doi.org/10.1016/j.ijfatigue.2015.12.003>
- Liu F, He C, Chen Y, et al (2020) Effects of defects on tensile and fatigue behaviors of selective laser melted titanium alloy in very high cycle regime. *Int J Fatigue* 140:105795. <https://doi.org/10.1016/j.ijfatigue.2020.105795>

- Masuo H, Tanaka Y, Morokoshi S, et al (2018) Influence of defects, surface roughness and HIP on the fatigue strength of Ti-6Al-4V manufactured by additive manufacturing. *Int J Fatigue* 117:163–179. <https://doi.org/10.1016/j.ijfatigue.2018.07.020>
- Meneghetti G, Rigon D, Cozzi D, et al (2017) Influence of build orientation on static and axial fatigue properties of maraging steel specimens produced by additive manufacturing. *Procedia Struct Integr* 7:149–157. <https://doi.org/10.1016/j.prostr.2017.11.072>
- Mooney B, Kourousis KI, Raghavendra R (2019) Plastic anisotropy of additively manufactured maraging steel: Influence of the build orientation and heat treatments. *Addit Manuf* 25:19–31. <https://doi.org/10.1016/j.addma.2018.10.032>
- Moretini G, Javad Razavi SM, Zucca G (2019) Effects of build orientation on fatigue behavior of Ti-6Al-4V as-built specimens produced by direct metal laser sintering. *Procedia Struct Integr* 24:349–359. <https://doi.org/10.1016/j.prostr.2020.02.032>
- Murakami Y (2019) *Metal fatigue : effects of small defects and nonmetallic inclusions*, II edition. Elsevier
- Murakami Y, Takagi T, Wada K, Matsunaga H (2021) Essential structure of S-N curve: Prediction of fatigue life and fatigue limit of defective materials and nature of scatter. *Int J Fatigue* 146:106138. <https://doi.org/10.1016/j.ijfatigue.2020.106138>
- Pellizzari M, AlMangour B, Benedetti M, et al (2020) Effects of building direction and defect sensitivity on the fatigue behavior of additively manufactured H13 tool steel. *Theor Appl Fract Mech* 108:102634. <https://doi.org/10.1016/j.tafmec.2020.102634>
- Qian G, Li Y, Paolino DS, et al (2020) Very-high-cycle fatigue behavior of Ti-6Al-4V manufactured by selective laser melting: Effect of build orientation. *Int J Fatigue* 136:105628. <https://doi.org/10.1016/j.ijfatigue.2020.105628>
- Razavi SMJ, Van Hooreweder B, Berto F (2020) Effect of build thickness and geometry on quasi-static and fatigue behavior of Ti-6Al-4V produced by Electron Beam Melting. *Addit Manuf* 36:101426. <https://doi.org/10.1016/j.addma.2020.101426>
- Rigon D, Meneghetti G (2020) An engineering estimation of fatigue thresholds from a microstructural size and Vickers hardness: application to wrought and additively manufactured metals. *Int J Fatigue* 139:105796. <https://doi.org/10.1016/j.ijfatigue.2020.105796>
- Rigon D, Meneghetti G (2021) Engineering estimation of the fatigue limit of wrought and defective additively manufactured metals for different load ratios. *Int J Fatigue*
- Rigon D, Meneghetti G, Görtler M, et al (2018) Influence of defects on axial fatigue strength of maraging steel specimens produced by additive manufacturing. *MATEC Web Conf* 165:02005. <https://doi.org/10.1051/mateconf/201816502005>
- Romano S, Nezhadfar PD, Shamsaei N, et al (2020) High cycle fatigue behavior and life prediction for additively manufactured 17-4 PH stainless steel: Effect of sub-surface porosity and surface roughness. *Theor Appl Fract Mech* 106:102477. <https://doi.org/10.1016/j.tafmec.2020.102477>
- Sadananda K, Nani Babu M, Vasudevan AK (2019) The unified approach to subcritical crack growth and fracture. *Eng Fract Mech* 212:238–257. <https://doi.org/10.1016/J.ENGFRACMECH.2019.03.010>
- Solberg K, Berto F (2019) Notch-defect interaction in additively manufactured Inconel 718. *Int J Fatigue* 122:35–45. <https://doi.org/10.1016/J.IJFATIGUE.2018.12.021>
- Wang Z, Palmer TA, Beese AM (2016) Effect of processing parameters on microstructure and tensile properties of austenitic stainless steel 304L made by directed energy deposition additive manufacturing. *Acta Mater* 110:226–235. <https://doi.org/10.1016/j.actamat.2016.03.019>
- Wycisk E, Solbach A, Siddique S, et al (2014) Effects of defects in laser additive manufactured Ti-6Al-4V on fatigue properties. *Phys Procedia* 56:371–378. <https://doi.org/10.1016/j.phpro.2014.08.120>
- Xu W, Brandt M, Sun S, et al (2015) Additive manufacturing of strong and ductile Ti-6Al-4V by selective laser melting via in situ martensite decomposition. *Acta Mater* 85:74–84. <https://doi.org/10.1016/j.actamat.2014.11.028>
- Yoder G, Cooley L, Crooker T (1983) A Critical Analysis of Grain-Size and Yield-Strength Dependence of Near-Threshold Fatigue Crack Growth in Steels. In: *Fracture Mechanics: Fourteenth Symposium—Volume I: Theory and Analysis*. ASTM International, 100 Barr Harbor Drive, PO Box C700, West Conshohocken, PA 19428-2959, pp I-348-I-348–18
- Zerbst U, Bruno G, Buffiere J-Y, et al (2021) Damage tolerant design of additively manufactured metallic components subjected to cyclic loading: State of the art and challenges. *Prog Mater Sci* 100786. <https://doi.org/10.1016/j.pmatsci.2021.100786>