

## Texture-based optimization of crystal plasticity parameters. Application to Zinc and its alloy.

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### Supplementary material

We present here an additional sensitivity analysis for Zn-1.5Mg alloy. As the same model was used for both materials studied in the main part of the paper, we believe that similar conclusions would be drawn in the case of pure zinc.

#### S.1. $n$ and $\dot{\gamma}_0$ sensitivity of Zn-1.5Mg alloy.

As the rate sensitivity of zinc and its alloy were neglected in the identification procedure, we have carried out an additional analysis. The VPSC code enables to account for the rate sensitivity effect or to neglect it. In the latter case, the strain rate at a grain level is scaled to the norm of the macroscopic strain rate. This option itself has no influence on the activity of slip systems or the evolution of texture, only the stress level is affected [30]. In the main part of the article we were concerned solely with texture evolution and thus we could safely use rate-insensitive option in VPSC. However, specifying the exact plastic strain rate (same as in experiment) together with different choice of the rate sensitivity  $n$  and the reference slip velocity  $\dot{\gamma}_0$  could introduce some differences in texture evolution itself and thus affect the calibration procedure.

In the analysis presented here, we have specified the realistic plastic strain rate (as applied in the experiment, cf. [9]) to be 6.82 and 12.90 1/s for the first and second pass of HE applied to Zn-1.5Mg alloy. Fig. S.1 presents the sensitivity analysis of the influence of both  $n$  and  $\dot{\gamma}_0$  in this case. There is some influence of the  $n$  value (cf. Fig. S.1a) on the fitness. However, as we had no experimental data concerning the rate-sensitivity of the material studied, we could not determine what would be the most appropriate  $n$  value and thus we took the one which offered good predictions in case of other hexagonal close-packed materials, cf. e.g. [1-4]. In Fig. S.1b, it can be clearly seen that the fitness values are almost insensitive to the value of  $\dot{\gamma}_0$  in the investigated range.

#### S.2. Sensitivity analysis for the optimized parameters (Zn-1.5Mg alloy)

In order to investigate the possible indeterminacy of the parameters, we have carried out a quasi-sensitivity analysis. We were not able to perform a full sensitivity analysis with evaluation of the derivatives of the fitness function. Therefore, we simply computed the fitness values while changing each of 42 parameters and keeping the remaining parameters unchanged. The parameters were changed so that they still lay in the prescribed range of parameters. Note that the simulation did not converge for every value of each parameter, that why some empty places appear in plots presented in Figs. S.2-S.5.

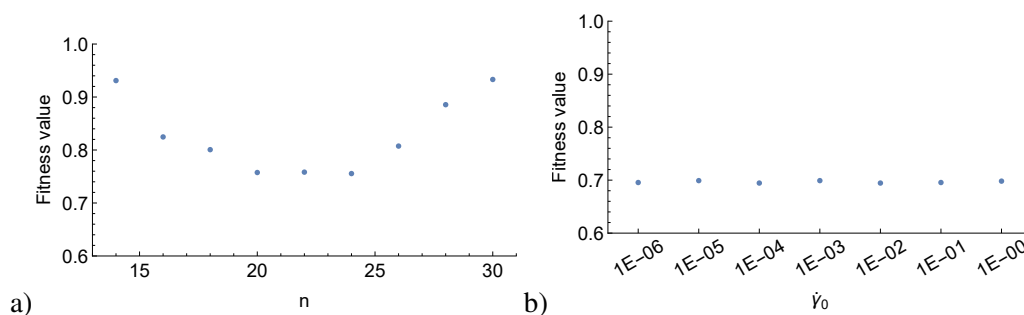


Figure S.1: Sensitivity analysis for a)  $n$  and b)  $\dot{\gamma}_0$ .

From the conducted analysis we can conclude that using the proposed fitness function, the values of  $\tau_0$ ,  $\tau_{sat}$ ,  $f_{sat}$  and  $\mu$  can be established with reasonable accuracy. On the other hand, the values of  $\beta$ ,  $h_0$  and latent hardening parameters cannot be really determined unambiguously using the proposed technique. Some additional experimental data are necessary to provide unambiguous values of the latter parameters.

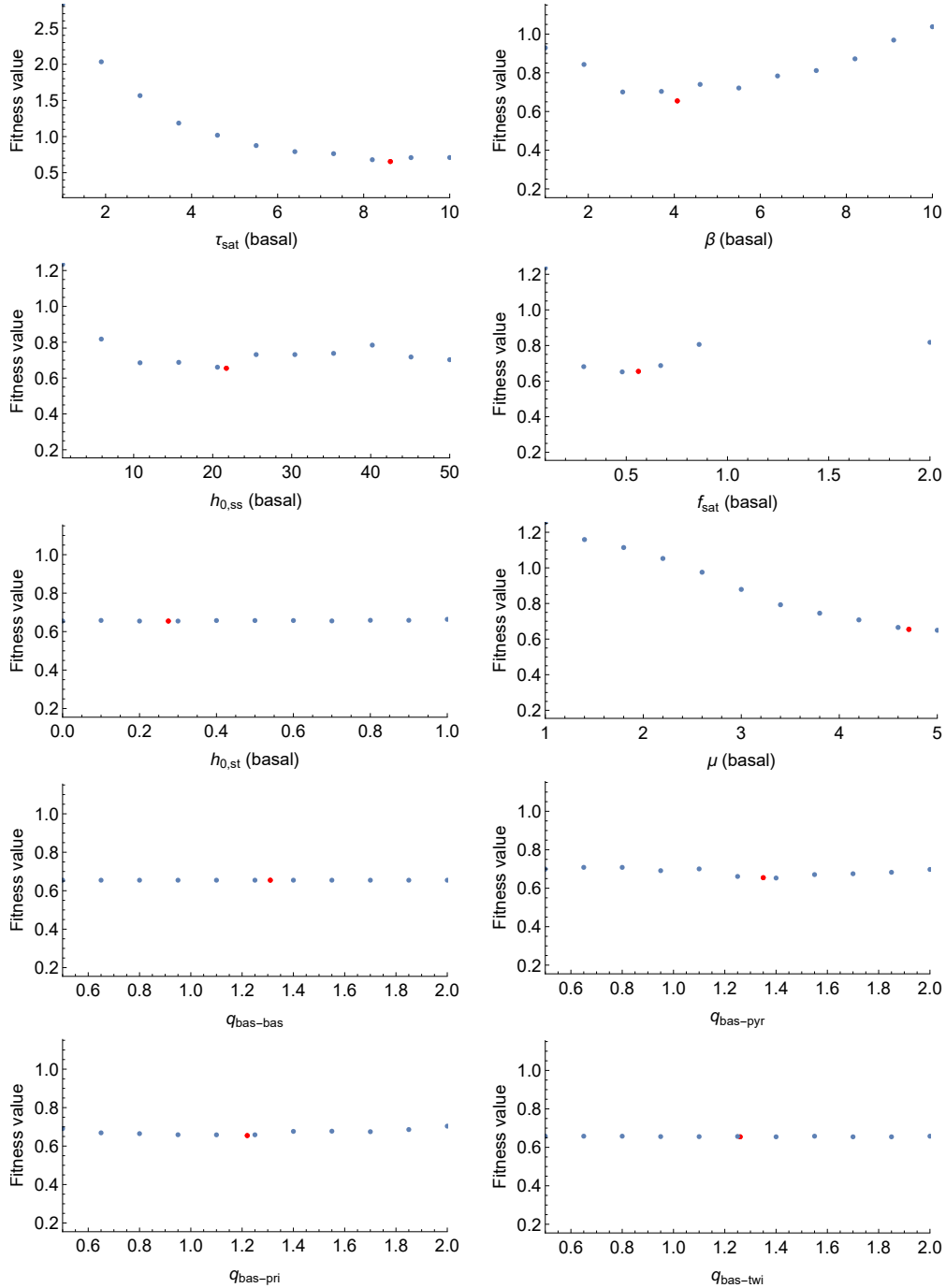


Figure S.2: Sensitivity analysis for the basal slip system

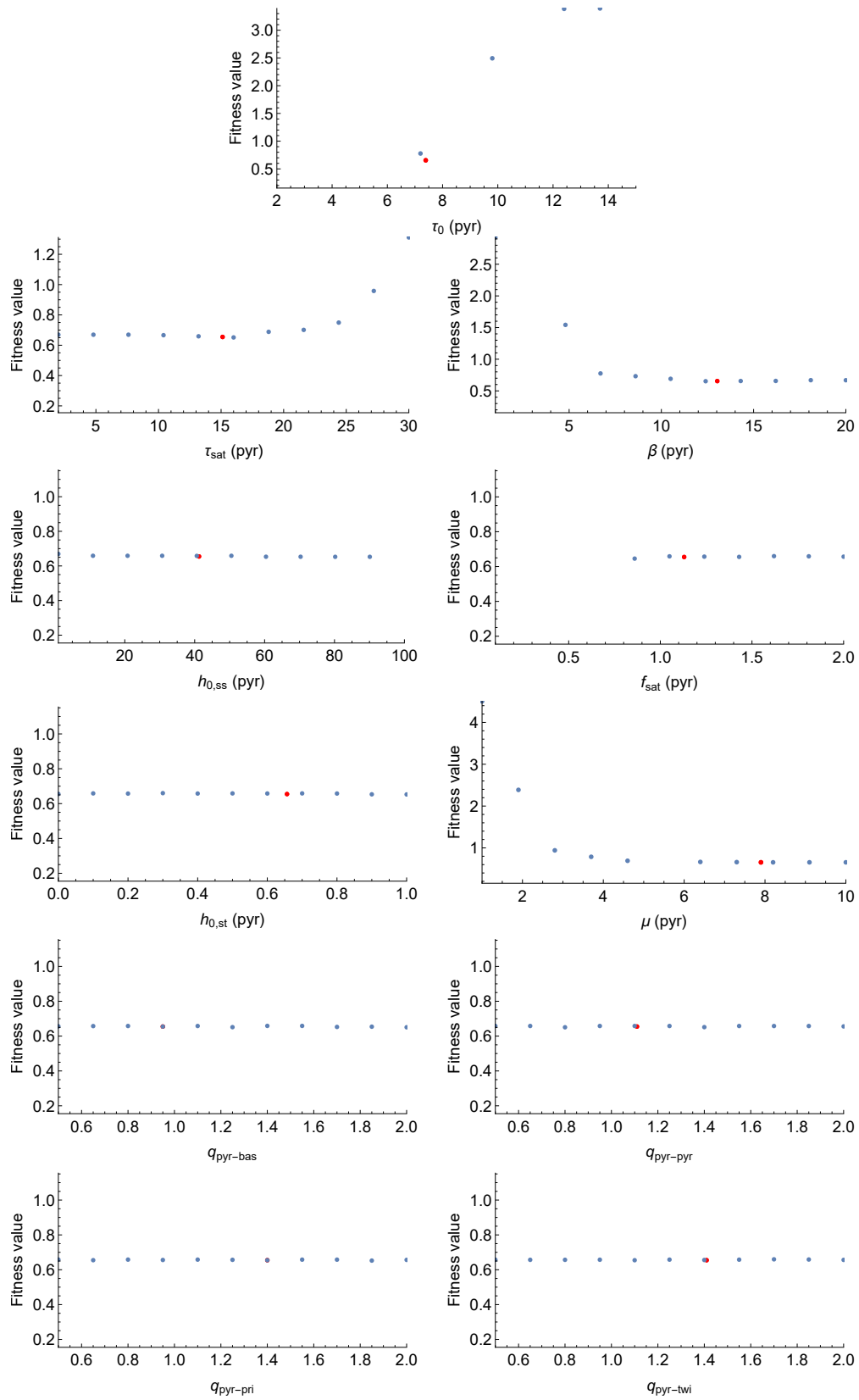


Figure S.3: Sensitivity analysis for the pyramidal  $\langle c+a \rangle$  slip system

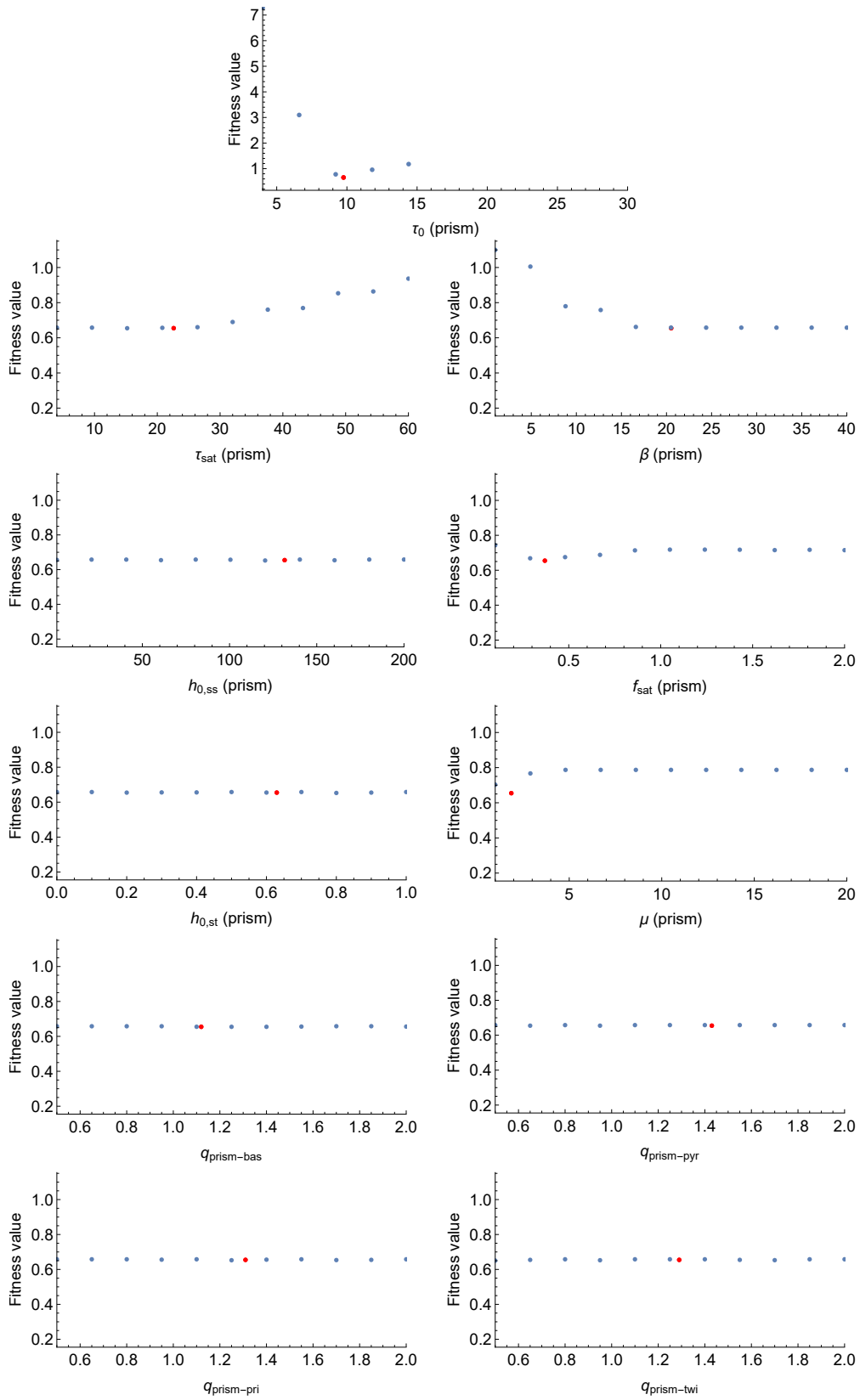


Figure S.4: Sensitivity analysis for the prismatic slip system

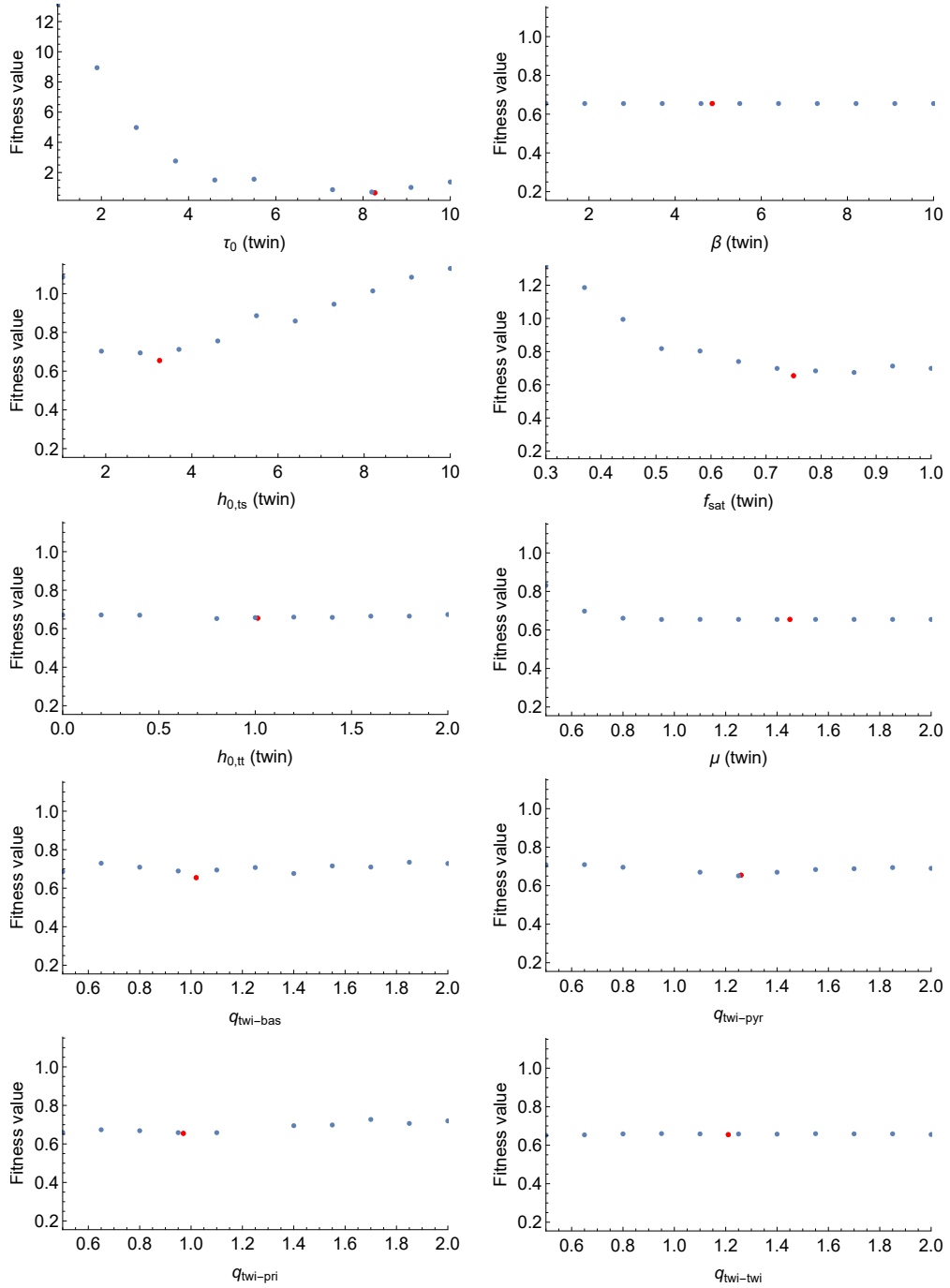


Figure S.5: Sensitivity analysis for twinning.