

Supplementary material

Table S1. Calculated parameters of  $\beta$ -(Zr, Nb).

№	at.% Nb	$a, \text{Å}$	$E, \text{eV}$	Elastic constants $C_{ij}$ (GPa)			$C_{11} - C_{12}$	$\Gamma$ (300 K)
				$C_{11}$	$C_{12}$	$C_{44}$		
1	0.0	3.573	8.44	81.9	91.2	30.1	-9.3	0.96
2	12.5	3.554	8.67	108.2	88.7	25.1	16.0	1.10
3	25.0	3.518	8.88	120.1	87.6	30.6	30.5	1.20
4	37.5	3.481	9.08	133.7	92.7	28.3	39.4	1.25
5	50.0	3.446	9.29	151.3	96.3	25.3	53.6	1.36
6	62.5	3.410	9.51	172.0	103.7	24.2	70.0	1.50
7	75.0	3.375	9.74	197.2	110.0	21.5	89.0	1.55
8	87.5	3.341	9.97	223.4	119.5	19.5	105.3	1.52
9	100.0	3.308	10.22	248.4	132.9	14.4	115.5	1.60

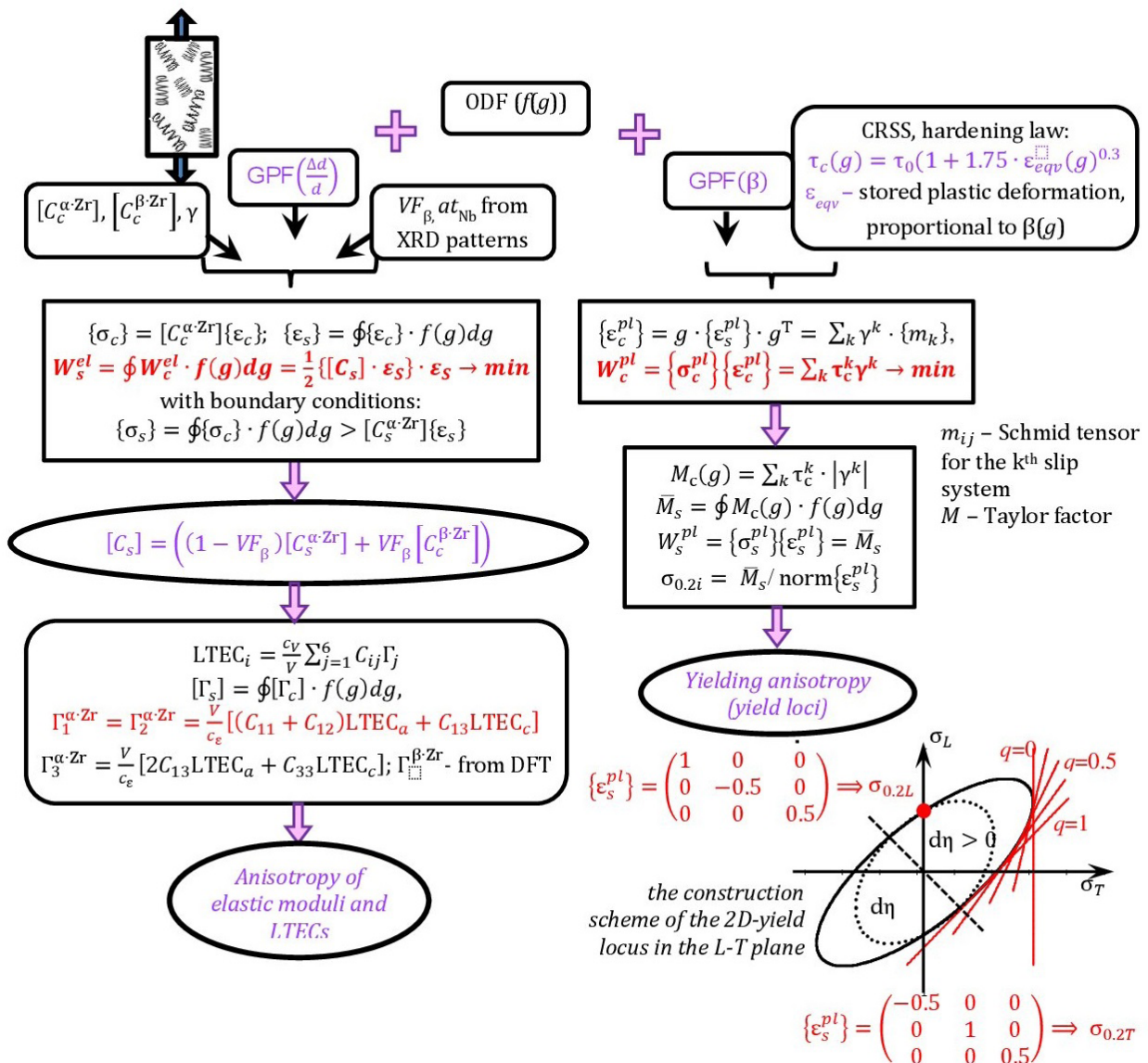


Fig. S1. (Color online) The generalized calculation algorithm of the properties anisotropy on the basis of GPFs data for elastic moduli and LTECs (a) and yield anisotropy (b).

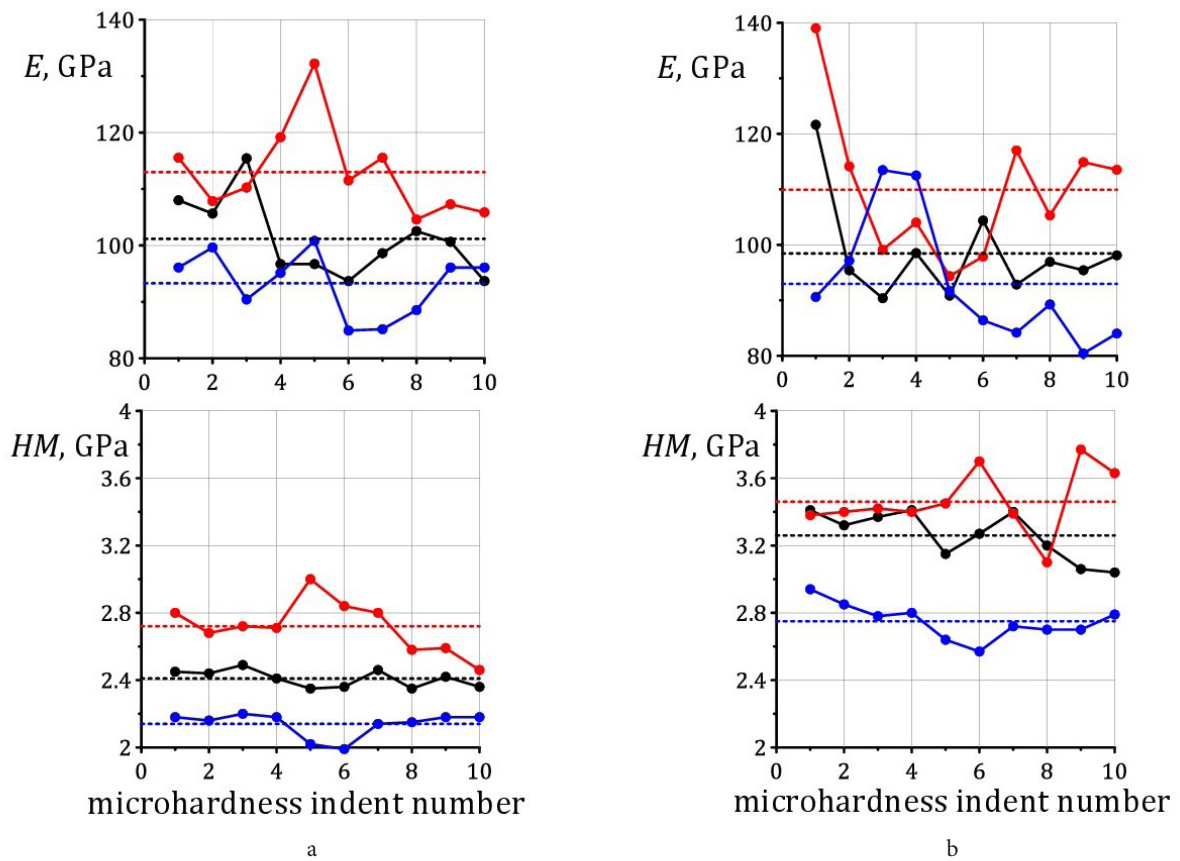


Fig. S2. (Color online) Indentation parameters obtained for different directions of the deformed (a) and annealed (b) samples.

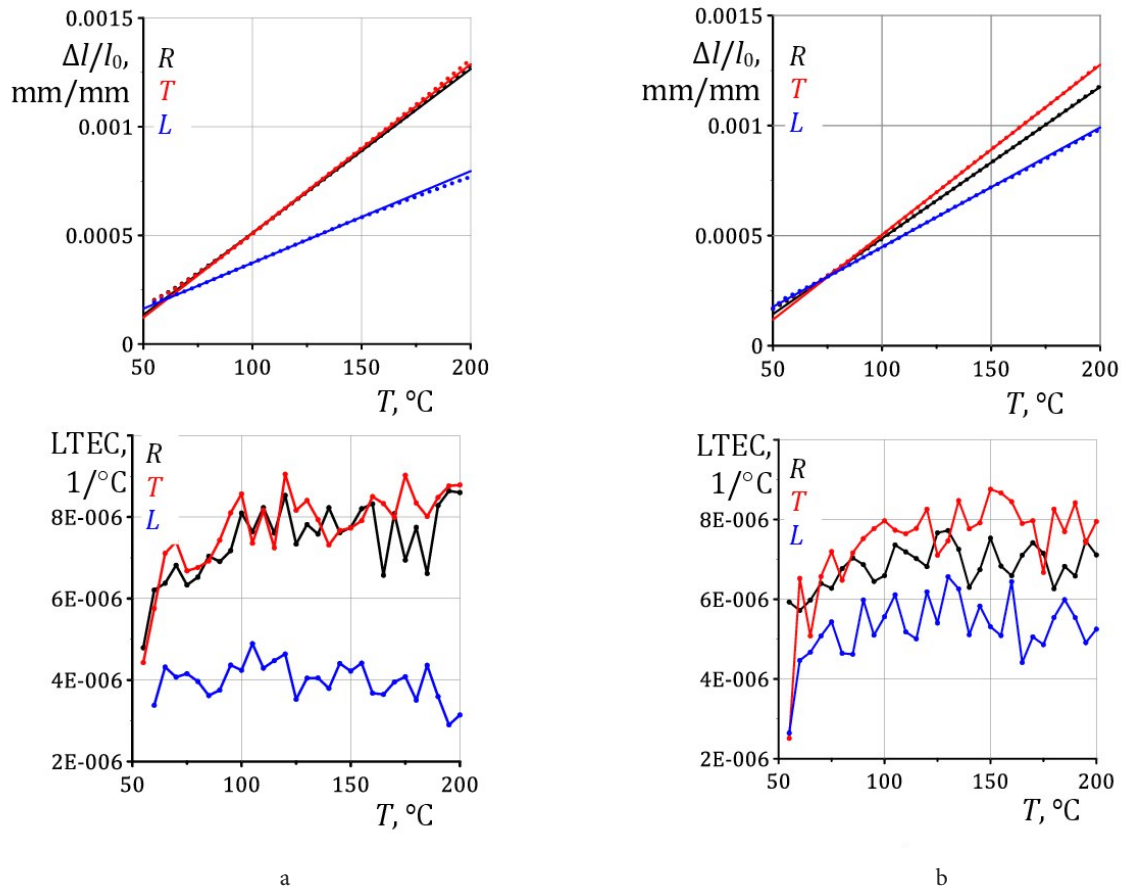
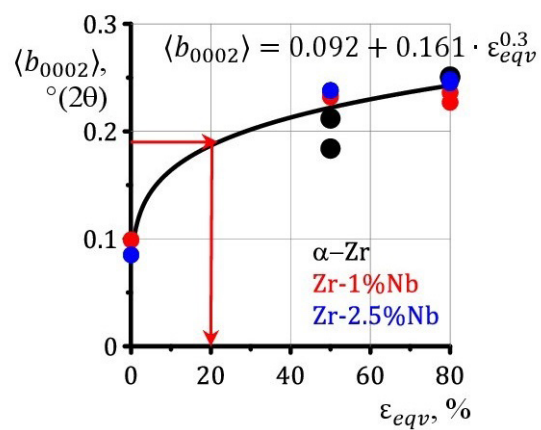


Fig. S3. (Color online) Dilatometric curves and appropriate LTECs, calculated every 5°, obtained for different directions of the deformed (a) and annealed (b) samples.



**Fig. S4.** (Color online) The dependency of the weighted average value  $\langle b_{0002} \rangle$  on accumulated degree of plastic deformation during rolling for pure Zr and different Zr-Nb alloys.