

Method for Controlling the Diameter of a Single Crystal to a Set Point Diameter

5 The invention relates to a method for controlling the diameter of a single crystal to a set point diameter during the pulling of the single crystal from a melt which is contained in a crucible.

10 The CZ method is a method which is used on the industrial scale, in order for example to produce silicon single crystals which are processed further to form wafers. The wafers are needed as substrates for the production of electronic components. In order to produce a silicon single crystal by the
15 CZ method, silicon is melted in a crucible, and a seed crystal is immersed in the melt and raised out from the melt. After the elimination of dislocations, the desired single crystal grows at the lower end of the seed crystal. The growth of the single crystal comprises a starting phase and an end phase, during
20 which the diameter of the single crystal is increased and decreased, respectively. This is normally done by changing the lift rate with which the seed crystal is raised. During a phase between the starting phase and the end phase, efforts are made to keep the diameter of the single crystal as constant as
25 possible, because only the section of the single crystal which is pulled during this phase is processed further to form wafers.

At the phase boundary on the edge of the single crystal, the
30 melt forms a meniscus. The meniscus is a region in which the melt extends downward with a particular curvature from the phase boundary on the edge of the single crystal to the level of a surface of the melt outside the meniscus. The outer edge of the meniscus is the place where the meniscus reaches the
35 level of the surface of the melt. The height of the meniscus is

the vertical distance between the phase boundary and the level of the surface of the melt outside the meniscus. The phase boundary on the edge of the single crystal is the place where the growing single crystal, the melt and the surrounding
 5 atmosphere meet. A tangent to this phase boundary and to the meniscus makes an angle with the vertical, the value of which depends on the height of the meniscus.

Under ideal conditions, which represent cylindrical growth of
 10 the single crystal with a constant set point diameter of the single crystal, the single crystal grows with a growth rate which corresponds to the value of the lift rate, but is opposite to the direction of the lift rate. Under these conditions, the height of the meniscus corresponds to the
 15 height z_0 . The angle between the tangent to the meniscus and to the phase boundary and the vertical has the value β_0 under these conditions.

If the height z of the meniscus or the meniscus angle β
 20 deviates from z_0 or β_0 , respectively, the single crystal will grow inward or outward and the actual diameter D_{cr} of the single crystal will deviate from the set point diameter. With $z > z_0$, or $\beta < \beta_0$, the derivative of the diameter with respect to time will be $dD_{cr}/dt < 0$, or vice versa.

25 Various methods for controlling the diameter of a single crystal are known. For example, they may be distinguished by the variable manipulated for the control. In this context, control by means of the manipulated variable lift rate v_p or
 30 the manipulated variable electrical power L_r of a heat source, which annularly encloses the single crystal, are to be highlighted. Both variants have the advantage that deviations of the diameter of the single crystal from the set point diameter can be reacted to with relatively fast response time.

JP1096089 A2, WO 01/57294 A1 and US 2011/0126757 A1 contain examples of these methods.

US 2009/0064923 A1 describes a method in which the height of
5 the meniscus is used in order to control the diameter, the
height of the meniscus being derived by evaluating the
brightness distribution in the course of the observation of a
bright ring. The bright ring is a reflection on the meniscus,
which is caused by neighboring components of the device for
10 pulling the single crystal being reflected in the meniscus.
Such components are in particular the crucible wall and the
lower end of a heat shield, which usually encloses the single
crystal, and, if present, a heat source which annularly
encloses the single crystal. According to US 2009/0064923 A1,
15 it is assumed that the position with the greatest brightness on
the bright ring represents the location of the phase boundary
on the edge of the single crystal, and the level of the surface
of the melt outside the meniscus can be detected by means of
the observed brightness distribution.

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This assumption, however, is only an approximation of the
physical situation. Furthermore, the fact that a short-term
change in the height of the meniscus has no significant effect
on the growth rate of the single crystal remains ignored.
25 Accordingly, control of the diameter of the single crystal on
the basis of the aforementioned method is inaccurate.

It is an objective of the present invention to provide an
improved method for controlling the diameter of a single
30 crystal to a set point diameter, which involves smaller changes
of the manipulated variable used for the control.

The object is achieved by a method for controlling the diameter
of a single crystal to a set point diameter during the pulling
35 of the single crystal from a melt, which is contained in a

crucible and forms a meniscus at a phase boundary on the edge of the single crystal, the meniscus having a height which corresponds to the distance between the phase boundary and a level of the surface of the melt outside the meniscus,

5 comprising repeated conduct of the following steps:
 determination of the diameter of a bright ring on the meniscus;
 calculation of a diameter of the single crystal while taking into account the diameter of the bright ring and while taking into account the dependency of the diameter of the bright ring
 10 on the height of the meniscus and on the diameter of the single crystal itself; and
 calculation of at least one manipulated variable for controlling the diameter of the single crystal on the basis of the difference between the calculated diameter of the single
 15 crystal and the set point diameter of the single crystal.

The aforementioned steps are carried out repeatedly, in which case the time intervals between the repetitions may be the same, although they need not be the same. As manipulated
 20 variables of the control, the lift rate v_p or the electrical power L_r of a heat source which annularly encloses the growing single crystal, or both, may preferably be envisioned.

The method is preferably used for the production of silicon
 25 single crystals.

The growth rate v_{cr} of the single crystal and the difference $\Delta\beta(z) = (\beta(z) - \beta_0)$ are the crucial variables which cause changes in the diameter of the single crystal as a function of time:

$$30 \quad \frac{dD_{cr}}{dt} = v_{cr} \times 2 \tan \Delta\beta(z) \quad (1)$$

The difference $\Delta\beta$ between the meniscus angles β and β_0 depends on the height z of the meniscus.

The growth rate v_{cr} of the single crystal is dictated primarily by the temperature field at the crystallization boundary. It is therefore influenced essentially by the electrical power L_f of a heat source which is arranged around the crucible, as well as by temperature variations in the melt as a result of the heat supply by the heat source.

A change in the height z of the meniscus as a function of time is given according to Equation (2), it being assumed that the lowering of the level of the surface of the melt due to the decrease in the volume of the melt because of the growth of the single crystal is compensated for exactly by the raising of the crucible:

$$dz/dt = v_p - v_{cr} \quad (2)$$

If this is not the case, then the difference between the rate of the change in the level of the surface and the rate of the crucible movement must be added to the right-hand side of the equation.

A change in the lift rate v_p has the direct effect that the height z of the meniscus and the meniscus angle β also change. The growth rate initially remains uninfluenced by such a change in the lift rate v_p . The invention takes into account this and the fact that the diameter of the bright ring depends on the diameter of the single crystal and on the height of the meniscus. If higher-order terms of a series expansion are neglected, the diameter D_{br} of the bright ring and the diameter D_{cr} of the growing crystal are interrelated by Equation (3).

$$D_{br} = D_{cr} + f_{cr}(D_{cr}) + f_z(z) \quad (3)$$

Accordingly, two further terms are of importance for the calculation of D_{cr} , namely a component $f_{cr}(D_{cr})$ relating to the

diameter of the bright ring, the value of which depends on the diameter of the single crystal and therefore on the radial position of the meniscus, and a component $f_z(z)$ relating to the diameter of the bright ring, the value of which depends on the height of the meniscus and therefore on the shape of the meniscus.

If Equation (3) is differentiated with respect to time, Equation (4b) is obtained via Equation (4a) by rearrangement, and Equation (5) is obtained by substituting Equation (1) and Equation (2) into Equation (4b).

$$\frac{dD_{br}}{dt} = \frac{dD_{cr}}{dt} + \frac{df_{cr}(D_{cr})}{dt} + \frac{df_z(z)}{dt} \quad (4a)$$

$$\frac{dD_{br}}{dt} = \frac{dD_{cr}}{dt} + \frac{df_{cr}(D_{cr})}{dD_{cr}} \times \frac{dD_{cr}}{dt} + \frac{df_z(z)}{dz} \times \frac{dz}{dt} \quad (4b)$$

$$\frac{dD_{br}}{dt} = \left(1 + \frac{df_{cr}(D_{cr})}{dD_{cr}}\right) \times v_{cr} \times Z \tan \Delta \beta(z) + \frac{df_z(z)}{dz} \times (v_p - v_{cr}) \quad (5)$$

15

It may be assumed that the growth rate v_{cr} corresponds to a set point value of the lift rate v_{ps} , and that $df_{cr}(D_{cr})/dD_{cr} = df_{cr}(D_{crs})/dD_{cr}$ for small changes in the diameter of the crystal, where D_{crs} stands for the set point diameter of the single crystal. Instead of this, however, the term $df_{cr}(D_{cr})/dD_{cr}$ may also be calculated iteratively.

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According to the invention, Equation (5) is used as a basis in order first to determine the height z of the meniscus. It takes into account the change in the component relating to the diameter of the bright ring, which depends on the height of the meniscus, as a function of the change in the height of the meniscus, and weights it with a factor which depends on the lift rate v_p and the growth rate v_{cr} .

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In order to determine the diameter of the bright ring, the bright ring is observed and optically recorded, and the image is evaluated electronically at least at one point, preferably at least at three points. The three points are preferably
 5 uniformly distributed on a semicircle around the single crystal. The outer transition from dark to bright in the recorded image is interpreted as a part of a segment of a circle, the diameter of which corresponds to the diameter D_{br} of the bright ring. If the evaluation at different points gives
 10 different diameters, these are averaged to form a diameter of the bright ring.

The change in the diameter of the bright ring as a function of time dD_{br}/dt is obtainable by determination of the diameter of
 15 the bright ring and subsequent numerical differentiation with respect to time.

A preferred way of determining the height z of the meniscus on the basis of Equation (5) is using two look-up tables which are
 20 based on simulation data. They are compiled beforehand, that is to say before the pulling of the single crystal, and assign different heights z of the meniscus the corresponding values of $\tan\Delta\beta(z)$ and the corresponding values of $df_z(z)/dz$, respectively, at a spacing Δz of for example 0.1 mm, for
 25 example in the range of $1 \text{ mm} \leq z \leq 11 \text{ mm}$. The simulation (ray-tracing simulation) comprises the tracing of ray paths which, coming from a camera, strike the meniscus and are reflected there into the surroundings. The simulation takes into account the configuration of the "hot zone" which is used during the
 30 pulling of the single crystal, as well as the process conditions prevailing during the pulling of the single crystal. In particular, the position and shape of the heat shield, and optionally the position and shape of the heat source which encloses the growing single crystal, and the position of the
 35 camera which records the bright ring, are taken into account.

Simulation data which are based on a 2D approach are less accurate than those which are based on a 3D approach. It is therefore preferable to take this into account when compiling the look-up tables, and employ a 3D approach. In particular, the allocation of the values of $df_z(z)/dz$ at the spacing Δz therefore becomes more accurate. The 3D approach involves determination of the diameter of the bright ring, in a similar way to real image processing, by means of simulation which sets in spatial relation the position of evaluation points on the bright ring which lie outside the plane of the camera. In the plane of the camera lie the camera, the evaluation point on the bright ring placed closest to the camera position, and the axis along which the growing single crystal is raised.

The two look-up tables are combined to form a single look-up table $tab(z)$ in such a way that each height z is assigned the corresponding right-hand side of Equation (5), which is expressed by Equation (6):

$$tab(z) = \left(1 + \frac{df_{cr}(D_{cr})}{dD_{cr}}\right) \times v_{cr} \times 2 \tan \Delta \beta(z) + \frac{df_z(z)}{dz} \times (v_p - v_{cr}) \quad (6)$$

During the pulling of the single crystal, the common look-up table $tab(z)$ is employed and, depending on the lift rate v_p and the growth rate v_{cr} , that value of z is interpolated which satisfies Equation (5) when the value that results from the differentiation of the diameter of the bright ring, which was determined beforehand, is used for the change in the diameter of the bright ring as a function of time dD_{br}/dt .

Another way of determining the associated height z of the meniscus on the basis of Equation (5) comprises simplification of Equation (5) by linearization of $\tan \Delta \beta(z)$ and $df_z(z)/dz$.

$$2 \tan \Delta \beta(z) \approx a_z + b_z \times z \quad (7)$$

$$df_z(z)/dz \approx a_m + b_m \times z \quad (8)$$

The coefficients a_t , b_t , a_m and b_m may for example be determined beforehand, that is to say before the pulling of the single crystal, by the method of least squares (least square fit).

- 5 After substitution of Equations (7) and (8) into Equation (5) and rearrangement, an expression which makes it possible to calculate the height z of the meniscus explicitly is obtained with Equation (9).

$$z = \frac{dD_{br}/dt - (1 + df_{cr}(D_{cr})/dD_{cr}) \times v_{cr} \times a_t - (v_p - v_{cr}) \times a_m}{(1 + df_{cr}(D_{cr})/dD_{cr}) \times v_{cr} \times b_t + (v_p - v_{cr}) \times b_m} \quad (9)$$

10

The value found according to Equation (6) or (9) for the height z of the meniscus is used in the next step in order to calculate the diameter D_{cr} of the single crystal according to Equation (10), which is derived from Equation (3), or in order
15 to calculate its derivative with respect to time dD_{cr}/dt according to Equation (1). D_{crs} denotes the set point diameter of the single crystal.

$$D_{cr} = D_{crs} + \frac{(D_{br} - D_{crs} - f_z(z) - f_{cr}(D_{crs}))}{(1 + \frac{df_{cr}(D_{crs})}{dD_{cr}})} \quad (10)$$

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$$dD_{cr}/dt = v_{cr} \times 2 \tan \Delta \beta(z) \quad (1)$$

- With D_{cr} and dD_{cr}/dt , the input variables for the control of the diameter of the single crystal are available in corrected form, so that the dependencies of the diameter of the bright ring on
25 the height of the meniscus and on the diameter of the single crystal are taken into account.

As a controller for the control of the diameter of the single crystal, a PID controller or a state feedback control may preferably be envisioned.

- 5 When a PID controller is used, the difference $D_{cr}-D_{crs}$ as a system deviation $e(t)$ and the derivative $de(t)/dt$ as a component of the D element are introduced into the equation of the controller in order to calculate the manipulated variable $u(t)$. The derivative $de(t)/dt$ is determined numerically or,
10 preferably, calculated according to Equation (1). Equation (11) describes an ideal PID controller, k_p denoting the factor of the P gain, and T_i and T_D being the time constants of the I element and the D element, respectively:

$$u(t) = k_p \times \left(e(t) + \int \frac{1}{T_i} e(t) dt + T_D \frac{d}{dt} e(t) \right) \quad (11)$$

- 15 When a state feedback control is used, the manipulated variable $u(t)$ is calculated according to Equation (12), k_D and k_z denoting feedback factors of the state variables, and ΔD_{cr} and Δz respectively being the difference between the state variable (diameter D_{cr} of the single crystal or height z of the meniscus
20 z) and the associated set point value of the state variable (D_{crs} or z_s , respectively).

$$u(t) = k_D \Delta D_{cr}(t) + k_z \Delta z(t) \quad (12)$$

- In the starting phase and the end phase, during which the
25 diameter of the single crystal is increased and decreased, respectively, or in order to adapt the diameter of the single crystal to the set point diameter during the intermediate phase, z_s must be calculated according to Equation (13) with the aid of the set point diameter D_{crs} , which is specified as a
30 function of the length of the single crystal.

$$\frac{dD_{crs}}{dt} = v_{cr} \times 2 \tan \Delta \beta(z_s) \quad (13)$$

The following may preferably be envisioned as a manipulated variable $u(t)$ for adapting the diameter D_{cr} of the single crystal to the set point diameter D_{crs} : the lift rate v_p or the
 5 electrical power L_r of the heat source which annularly encloses the single crystal, or both.

In the case in which L_r is used as a manipulated variable, a predetermined set point lift rate v_{ps} is departed from as little
 10 as possible. The determination of the height z of the meniscus is carried out as already explained, but with Equation (14) being used, instead of the assumption $v_{cr} = v_{ps}$, in Equations (5), (6) and (9).

$$v_{cr} = v_{ps} + \frac{dv_{cr}}{dL_r} \times \Delta L_r \quad (14)$$

15

In this case, dv_{cr}/dL_r is preferably assumed to be constant and determined empirically. ΔL_r denotes the difference between the electrical power L_r of the heat source, which annularly
 encloses the single crystal, and its set point value L_{rs} .

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The manipulated variable $u(t)$ then calculated according to Equation (11) or (12) may then be converted into a corresponding manipulated variable $u_{Lr}(t)$. For the conversion, a factor which converts $u(t)$ into $u_{Lr}(t)$ is determined
 25 empirically. The manipulated variable $u_{Lr}(t)$ corresponds to the change in the electrical power ΔL_r of the heat source which is necessary in order to cause a change in the growth rate which brings the diameter D_{cr} of the single crystal close to the set point diameter.

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It is recommendable, and therefore preferred, to filter variables affected by measurement noise before use as calculation variables in the corresponding equations. This applies in particular for the following variables: the diameter
5 D_{br} of the bright ring, the height z of the meniscus, the lift rate v_p , and the electrical power L_r of the heat source which encloses the growing single crystal. A PT1 filter with an adjustable time constant is preferably used for the filtering.

10 It is furthermore advantageous, and therefore also preferred, besides the described control of the diameter of the single crystal, to establish a further control loop, which reacts in the event of deviations of the lift rate v_p from the set point lift rate v_{ps} or deviations of the electrical power L_r from the
15 set point power L_{rs} , and the manipulated variable of which modifies the electrical power L_f of at least one heat source which is arranged around the crucible. The further control loop therefore relieves the load on the single crystal diameter control according to the invention.

20 The invention will be described below with reference to drawings.

Fig. 1 shows the vicinity of the phase boundary between the
25 growing single crystal, the melt and the surrounding atmosphere.

Fig. 2 shows the dependency of the diameter of the bright ring, and that of the meniscus angle, on the height of the meniscus.

30 Fig. 3 shows typical features of a device which is suitable for carrying out the method according to the invention.

Fig. 4 shows the profiles of the lift rate v_p and of the set point lift rate v_{ps} as a function of time, without and with control according to the invention.

5 As represented in Fig. 1, the melt rises toward the phase boundary TRP on the edge of the single crystal and forms a meniscus there. The phase boundary refers to the position where the liquid phase l of the melt, the solid phase s of the single crystal and the gaseous phase g of the atmosphere meet one
10 another. The height z of the meniscus is the vertical separation between the phase boundary TRP and the level ML of the surface of the melt outside the meniscus.

The tangent to the phase boundary and to the meniscus makes the
15 meniscus angle β with the vertical, the value of which depends on the height of the meniscus. The single crystal is pulled with a lift rate v_p from the melt and grows with a growth rate v_{cr} in the opposite direction. If the single crystal grows with a constant set point diameter D_{crs} , then $\beta = \beta_0$, $z = z_0$ and $v_p =$
20 v_{cr} . Such conditions are ideal for pulling the section of the single crystal which is subsequently intended to be processed further to form wafers.

In the event of deviations $\Delta z \neq 0$ ($\Delta z = z - z_0$), or $\Delta \beta \neq 0$ ($\Delta \beta = \beta - \beta_0$), the single crystal starts to grow inward or outward
25 and the diameter D_{cr} of the single crystal starts to deviate from the set point diameter D_{crs} . In the case of $z > z_0$ and $\beta < \beta_0$, the diameter of the single crystal becomes smaller ($dD_{cr}/dt < 0$), and vice versa.

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As shown in Fig. 2, there is a nonlinear dependency between the diameter of the bright ring and the height of the meniscus ($\Delta D_{br} = D_{br}(z) - D_{br}(z_0)$). Likewise represented are the

corresponding dependencies of the terms $2\tan\Delta\beta(z)$ and $df_z(z)/dz$ contained in Equation (5).

Fig. 3 shows typical features of a device which is suitable for carrying out the method according to the invention. The device comprises a crucible 1 which contains a melt 2, from which a single crystal 3 is pulled. A heat source 4, which keeps the melt liquid, is arranged around the crucible. An apparatus for generating a magnetic field, with which flows in the melt are influenced, is furthermore often provided. A further heat source 5 may be provided, which is arranged around the single crystal 3 and heats the region of a phase boundary between the single crystal, the melt and the surrounding atmosphere. The further heat source 5 may be used in order to control the diameter of the single crystal in the manner according to the invention. In this case, the manipulated variable of the control is aimed at influencing the electrical power L_r of the further heat source 5. Instead of the further heat source 5, an apparatus 6 for pulling the single crystal from the melt, which is only indicated in Fig. 3, may also be employed in order to control the diameter of the single crystal. The manipulated variable of the control is then aimed at influencing the lift rate v_p with which the single crystal is pulled upward from the melt. As an alternative to this, the electrical power L_r of the further heat source 5 and the lift rate v_p may be provided as manipulated variables of the control.

The volume of the melt 2 decreases with the growth of the single crystal 3, and therefore so does the level of the surface of the melt relative to the edge of the crucible. Conventionally, the crucible is raised in accordance with the volume loss of the melt so that the distance between the level ML of the surface of the melt and the lower edge of a heat shield 7, which encloses the growing single crystal, remains

unchanged. If maintenance of this distance is not kept constant, the decrease in the volume of the melt must also be taken into account in the calculation of the system of the control of the diameter of the single crystal.

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Further features of the device are at least one camera 8 for observing the melt 2 in the region of the meniscus and an image processing unit 9 for evaluating the image signal delivered by the camera. The evaluation comprises determination of the
10 diameter D_{br} of the bright ring and delivery thereof as input information for a compensator unit 10. There, the diameter D_{cr} of the single crystal is calculated in the manner according to the invention by using this input information and sent to a controller unit 11. A PID controller or a state feedback
15 control may preferably be envisioned as the controller unit 11. The controller unit 11 calculates the manipulated variable and makes it available to a control apparatus 12. Taking into account the manipulated variable, the control apparatus 12 undertakes the control of an electrical supply unit 13 for
20 supplying the heat sources with electricity, the control of a crucible displacement device 14 and the control of the apparatus 6 for pulling the single crystal from the melt.

The success of the invention can be seen from Fig. 4. This
25 shows the profiles of the lift rate v_p and of the set point lift rate v_{ps} as a function of time, without and with use of the control according to the invention. A silicon single crystal having a set point diameter of somewhat more than 300 mm was pulled. The profile of the lift rates reveals that, with the
30 incorporation of the compensator unit as indicated by an arrow, the outlay which is required in order to achieve adaptation of the diameter of the single crystal to the set point diameter by changes in the manipulated variable is significantly reduced.

Patent Claims

1. A method for controlling the diameter of a single crystal to a set point diameter during the pulling of the single crystal
5 from a melt, which is contained in a crucible and forms a meniscus at a phase boundary on the edge of the single crystal, the meniscus having a height which corresponds to the distance between the phase boundary and a level of the surface of the melt outside the meniscus, comprising repeated conduct of the
10 following steps:
determination of the diameter of a bright ring on the meniscus;
calculation of a diameter of the single crystal while taking into account the diameter of the bright ring and while taking into account the dependency of the diameter of the bright ring
15 on the height of the meniscus and on the diameter of the single crystal itself; and
calculation of at least one manipulated variable for controlling the diameter of the single crystal on the basis of the difference between the calculated diameter of the single
20 crystal and the set point diameter of the single crystal.
2. The method as claimed in claim 1, comprising the formation of a look-up table which is based on simulation data and allocates the height of the meniscus to the derivative of the
25 diameter of the bright ring as a function of time.
3. The method as claimed in claim 1, comprising calculation of the height of the meniscus from a linearized determination equation.
- 30 4. The method as claimed in one of claims 1 to 3, comprising calculation of the manipulated variable as an output variable of a PID controller.

5. The method as claimed in one of claims 1 to 3, comprising calculation of the manipulated variable as an output variable of a state feedback control.

5 6. The method as claimed in one of claims 1 to 5, wherein a lift rate is calculated as a manipulated variable.

7. The method as claimed in one of claims 1 to 5, wherein an electrical power of a heat source, which annularly encloses the
10 single crystal, is calculated as a manipulated variable.

8. The method as claimed in one of claims 1 to 7, wherein a lift rate is calculated as a first manipulated variable and an electrical power of a heat source, which annularly encloses the
15 single crystal, is calculated as a second manipulated variable.

9. The method as claimed in one of claims 1 to 8, comprising the establishment of a control loop which reacts in the event of deviations of the lift rate v_p from the set point lift rate v_{ps} or deviations of the electrical power L_r from the set point power L_{rs} , and the manipulated variable of which modifies the electrical power L_f of one or more heat sources which are arranged around the crucible.